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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) 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
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	272.755	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) 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
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

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

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) 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
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	16.78	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) 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
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

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) 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

BRUKER

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

Isotope		Spin	Nat. Abund. (%)	Receptivity		Larmor Frequencies (MHz) vs. Bruker Field Strengths (Tesla) 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
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); $\boldsymbol{\mu_z}$ = z-component of nuclear magnetic moment in units of the nuclear magneton (μ_N); ***Q*** = electric quadrupole moment in units of fm^2 = 10^{-30} m^2 (1 fm^2 = 0.01 barns); calc. magnetogyric ratio $\gamma = \mu_z/\hbar\, I$. Note: for $\boldsymbol{\mu_z}$ 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		-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_o calc. from γ and scaled to ^{1}H = 100.0 MHz; Molar Receptivity **R_M(H)** relative to equal number of protons is proportional to $\gamma^3 I(I+1)$; Receptivity at nat. abundance **R_{NA}(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 (^{1}H) = 100.0 MHz).
Numbers containing E are in exponential format.

		Theoretical NMR Freq. (free atom)	**Molar Receptivity** (rel. ^{1}H)	**Receptivity at Nat. Abund.** (rel. ^{13}C)	**Reference Sample**	**Measured. NMR Freq.** (rel. ^{1}H ref.)
A	**Sym**	ν_o [MHz]	**R_M(H)**	**R_{NA}(C)**	**Reference**	Ξ [MHz]
1	n	68.4979	3.21E–01			
1	H	100.0000	**1.00E+00**	5.87E+03	1% Me_4Si in $CDCl_3$	100.000000
2	D	15.3506	9.65E–03	6.52E–03	$(CD_3)_4Si$ 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_2O	14.716086
7	Li	38.8667	2.94E–01	1.59E+03	9.7 m LiCl in D_2O	38.863797
9	Be	14.0536	1.39E–02	8.15E+01	0.43 m $BeSO_4$ in D_2O	14.051813
10	B	10.7456	1.99E–02	2.32E+01	15% $BF_3.Et_2O$ in $CDCl_3$	10.743658
11	B	32.0897	1.65E–01	7.77E+02	15% $BF_3.Et_2O$ in $CDCl_3$	32.083974
13	C	25.1504	1.59E–02	**1.00E+00**	1% Me_4Si in $CDCl_3$ DSS in D_2O	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_2O	13.556457
19	F	94.0570	8.32E–01	4.89E+03	CCl_3F	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_2O	26.451900
25	Mg	6.1260	2.68E–03	1.58E+00	11 M $MgCl_2$ in D_2O	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_2O	26.056859
29	Si	19.8826	7.86E–03	2.16E+00	1% Me_4Si in $CDCl_3$	19.867187
31	P	40.5178	6.65E–02	3.91E+02	H_3PO_4 external $(MeO)_3PO$ internal	40.480742 40.480864
33	S	7.6842	2.27E–03	1.00E–01	$(NH_4)_2SO_4$ in D_2O (sat.)	7.676000
35	Cl	9.8093	4.72E–03	2.10E+01	0.1 M NaCl in D_2O	9.797909
37	Cl	8.1652	2.72E–03	3.88E+00	0.1 M NaCl in D_2O	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_2O	4.666373
40	K	5.8099	5.23E–03	3.59E–03	0.1 M KCl in D_2O	5.802018
41	K	2.5648	8.44E–05	3.34E–02	0.1 M KCl in D_2O	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_2O	6.730029
45	Sc	24.3299	3.02E–01	1.78E+03	0.06 M $Sc(NO_3)_3$ in D_2O	24.291747
47	Ti	5.6464	2.10E–03	9.18E–01	$TiCl_4$ neat + 10% C_6D_{12}	5.637534
49	Ti	5.6479	3.78E–03	1.20E+00	$TiCl_4$ neat + 10% C_6D_{12}	5.639037
50	V	9.9829	5.57E–02	8.18E–01	$VOCl_3$ + 5% C_6D_6	9.970309
51	V	26.3362	3.84E–01	2.25E+03	$VOCl_3$ + 5% C_6D_6	26.302948
53	Cr	5.6638	9.08E–04	5.07E–01	K_2CrO_4 in D_2O (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_2O	24.789218
57	Fe	3.2448	3.42E–05	4.25E–03	$Fe(CO)_5$ + 20% C_6D_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_2O	23.727074
60	Co	13.6026	1.01E–01			
61	Ni	8.9517	3.59E–03	2.40E–01	$Ni(CO)_4$ + 5% C_6D_6	8.936051
63	Cu	26.5839	9.39E–02	3.82E+02	$[Cu(CH_3CN)_4][ClO_4]$ in CH_3CN (sat.) + 5% C_6D_6	26.515473
65	Cu	28.4250	1.15E–01	2.08E+02	$[Cu(CH_3CN)_4][ClO_4]$ in CH_3CN (sat.) + 5% C_6D_6	28.403693
67	Zn	6.2675	2.87E–03	6.92E–01	$Zn(NO_3)_3$ in D_2O (sat.)	6.256803
69	Ga	24.0685	6.97E–02	2.46E+02	1.1 m $Ga(NO_3)_3$ in D_2O	24.001354
71	Ga	30.5813	1.43E–01	3.35E+02	1.1 m $Ga(NO_3)_3$ in D_2O	30.496704
73	Ge	3.4989	1.41E–03	6.44E–01	Me_4Ge + 5% C_6D_6	3.488315
75	As	17.1804	2.54E–02	1.49E+02	0.5 M $NaAsF_6$ in CD_3CN	17.122614
77	Se	19.1587	7.03E–03	3.15E+00	Me_2Se + 5% C_6D_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_o [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_2O	25.053980
81	Br	27.0997	9.95E–02	2.88E+02	0.01 M NaBr in D_2O	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_2O	9.654943
87	Rb	32.8436	1.77E–01	2.90E+02	0.01 M RbCl in D_2O	32.720454
87	Sr	4.3508	2.72E–03	1.12E+00	0.5 M $SrCl_2$ in D_2O	4.333822
89	Y	4.9203	1.19E–04	7.00E–01	$Y(NO_3)_3$ in H_2O/D_2O	4.900198
91	Zr	9.3354	9.49E–03	6.26E+00	$Zr(C_5H_5)_2Cl_2$ in CH_2Cl_2 (sat.) + 5% C_6D_6	9.296298
93	Nb	24.5488	4.88E–01	2.87E+03	$K[NbCl_6]$ in CH_3CN / CD_3CN (sat.)	24.476170
95	Mo	6.5467	3.27E–03	3.06E+00	2 M Na_2MoO_4 in D_2O	6.516926
97	Mo	6.6849	3.49E–03	1.96E+00	2 M Na_2MoO_4 in D_2O	6.653695
99	Mo	13.4272	2.42E–03			
99	Tc	22.6161	3.82E–01		NH_4TcO_4 in H_2O / D_2O	22.508326
99	Ru	4.5903	1.13E–03	8.46E–01	0.3 M $K_4[Ru(CN)_6]$ in D_2O	4.605151
101	Ru	5.1274	1.57E–03	1.58E+00	0.3 M $K_4[Ru(CN)_6]$ in D_2O	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_2PdCl_6 in D_2O (sat.)	4.576100
107	Ag	4.0704	6.74E–05	2.05E–01	$AgNO_3$ in D_2O (sat.)	4.047819
109	Ag	4.6795	1.02E–04	2.90E–01	$AgNO_3$ in D_2O (sat.)	4.653533
111	Cd	21.3003	9.66E–03	7.27E+00	Me_2Cd neat liq.	21.215480
113	Cd	22.2820	1.11E–02	7.94E+00	Me_2Cd neat liq.	22.193175
113	In	21.9963	3.51E–01	8.85E+01	0.1 M $In(NO_3)_3$ in D_2O + 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_2O + 0.5 M DNO_3	21.912629
115	Sn	32.8994	3.56E–02	7.11E–01	Me_4Sn + 5% C_6D_6	32.718749
117	Sn	35.8430	4.60E–02	2.08E+01	Me_4Sn + 5% C_6D_6	35.632259
119	Sn	37.4986	5.27E–02	2.66E+01	Me_4Sn + 5% C_6D_6	37.290632
121	Sb	24.0858	1.63E–01	5.48E+02	$KSbCl_6$ in CH_3CN / CD_3CN (sat.)	23.930577
123	Sb	13.0425	4.66E–02	1.17E+02	$KSbCl_6$ in CH_3CN / CD_3CN (sat.)	12.959217
125	Sb	13.4527	5.11E–02			
123	Te	26.3870	1.84E–02	9.61E–01	Me_2Te + 5% C_6D_6	26.169742
125	Te	31.8136	3.22E–02	1.34E+01	Me_2Te + 5% C_6D_6	31.549769
127	I	20.1462	9.54E–02	5.60E+02	0.01 M KI in D_2O	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_2O	13.116142
135	Ba	10.0092	5.01E–03	1.94E+00	0.5 M $BaCl_2$ in D_2O	9.934457
137	Ba	11.1874	7.00E–03	4.62E+00	0.5 M $BaCl_2$ in D_2O	11.112928
137	La	13.7852	5.50E–02			
138	La	13.2970	9.40E–02	4.97E–01	$LaCl_3$ in D_2O / H_2O	13.194300
139	La	14.2356	6.06E–02	3.56E+02	0.01 M $LaCl_3$ in D_2O	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 $Yb(\eta\text{-}C_5Me_5)_2(THF)_2$ 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_o [MHz]	$R_M(H)$	$R_{NA}(C)$	Reference	Ξ [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_3CN (sat.)	11.989600
183	W	4.2174	7.50E–05	6.31E–02	1 M Na_2WO_4 in D_2O	4.166387
185	Re	22.8233	1.39E–01	3.05E+02	0.1 M $KReO_4$ in D_2O	22.524600
187	Re	23.0568	1.43E–01	5.26E+02	0.1 M $KReO_4$ in D_2O	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_2PtCl_6 in D_2O	21.496784
197	Au	1.7683	2.76E–05	1.62E–01		
199	Hg	18.1136	5.94E–03	5.89E+00	Me_2Hg neat liq. (toxic!)	17.910822
201	Hg	6.6864	1.49E–03	1.16E+00	Me_2Hg 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_4Pb + 5% C_6D_6	20.920599
209	Bi	16.3525	1.44E–01	8.48E+02	$Bi(NO_3)_2$ sat. in conc. HNO_3 + 50% D_2O	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_6D_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/

NMR Tables

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	Manganese	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.

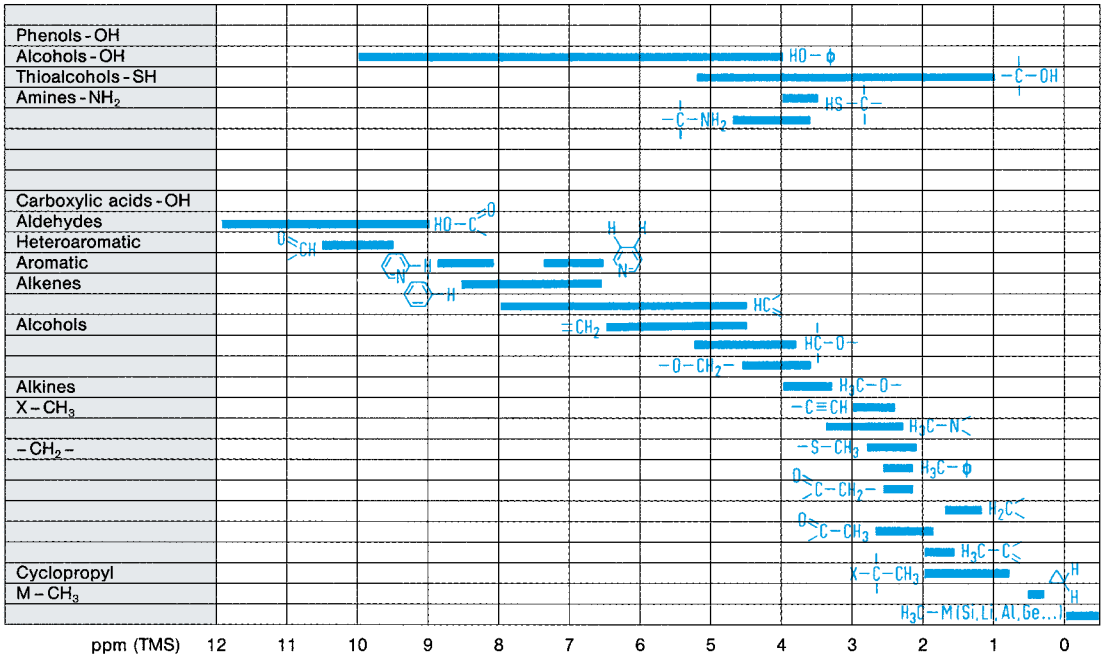
Properties of Selected Deuterated Solvents for NMR

Solvent	Formula	MW_{ave}	Density $[d_4^{20}]$	MP [°C]	BP [°C]	RI $[n_D^{20}]$	Dielec. [ε]	^{1}H shift (Mult.) [ppm]	J(HD) [Hz]	^{13}C Shift (Mult.) [ppm]	J(CD) [Hz]	H_2O/HDO Shift [ppm]
Acetic Acid-d4	$C_2D_4O_2$	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_3D_6O	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_2D_3N	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_6D_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	$C_6D_{12}O$	96.24	0.890	7	78		2	1.38		26.43 (5)	19	0.80
Deuterium oxide	D_2O	20.03	1.107	3.8	101.4	1.328	78.5	4.81				
1,2-Dichloroethane-d4	$C_2D_4Cl_2$	102.99	1.307	–35	83	1.443		3.72 (5)		43.6 (5)	23.5	
Dichloromethane-d2	CD_2Cl_2	86.95	1.362	–97	39.5	1.362		5.32 (3)	1.1	54 (5)	27.2	1.52
Diethylether-d10	$C_4D_{10}O$	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)	$C_6D_{14}O_3$	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)	$C_4D_{10}O_2$	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_3D_7NO	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_2D_6OS	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	$C_4D_8O_2$	96.16	1.129	12	99	1.4198	2.2	3.53 (m)		66.66 (5)	21.9	2.4
Ethanol-d6	C_2D_6O	52.11	0.888	–114.5	78	1.358	24.5	5.29 3.56 1.11 (m)		56.96 (5) 17.31 (7)	22 19	5.2
Methanol-d4	CD_4O	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_7D_{14}	112.27	0.77	–126	101	1.4189						
Nitrobenzene-d5	$C_6D_5NO_2$	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_3NO_2	64.06	1.19	–26	100	1.3795		4.33 (5)		62.8 (7)	22	2.2
2-Propanol-d8	C_3D_8O	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_5D_5N	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	$C_2D_2Cl_4$	169.86	1.7	–43	146	1.493		5.91 (5)		74.2 (5)		1.5
Tetrahydrofuran-d8	C_4D_8O	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_7D_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	$C_2DF_3O_2$	115.03	1.50	–15	71	1.30		11.50		164.2 (4) 116.6 (4)		11.5
2,2,2-Trifluoroethanol-d3	$C_2D_3F_3$	87.06	1.42	–44	77	1.30		5.02 3.88 (4x3)	2 (9)	126.3 (4) 61.5 (4x5)	22	5

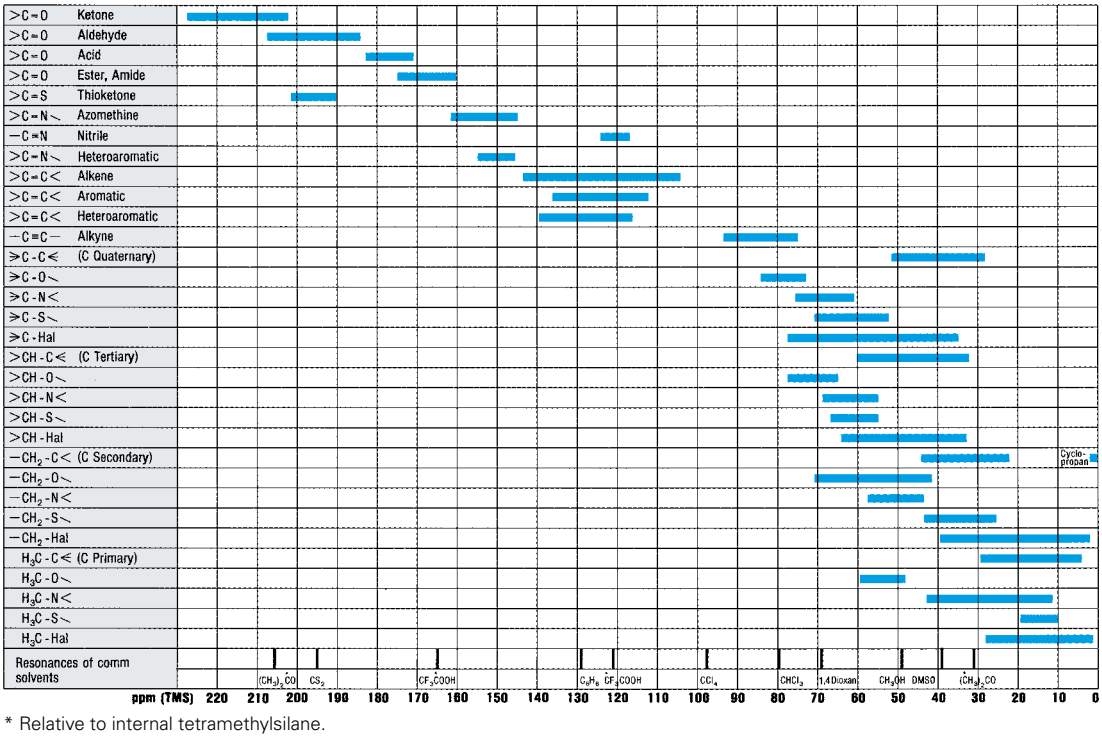
This Table summarizes the physical properties of deuterated solvents and the chem. shifts (rel. to TMS) and deuterium couplings for the solvent signals and the approximate shifts for residual water (last column).

NMR Tables

^{1}H Chemical Shifts in Organic Compounds



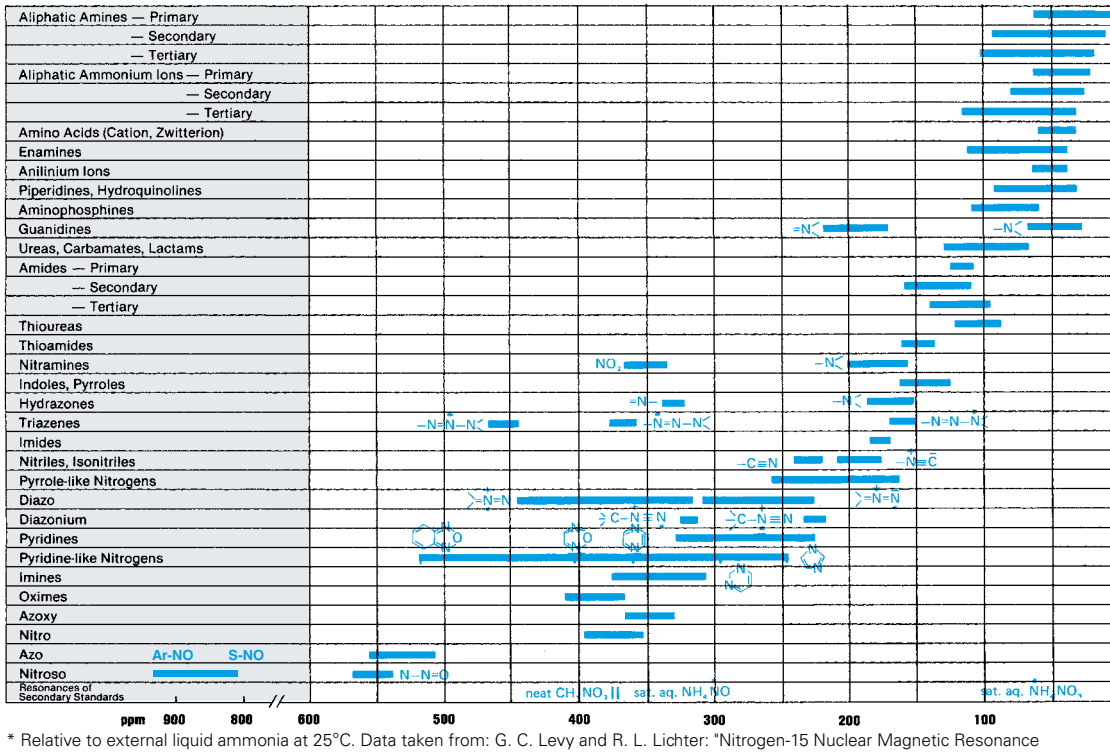
^{13}C Chemical Shifts in Organic Compounds*



* Relative to internal tetramethylsilane.

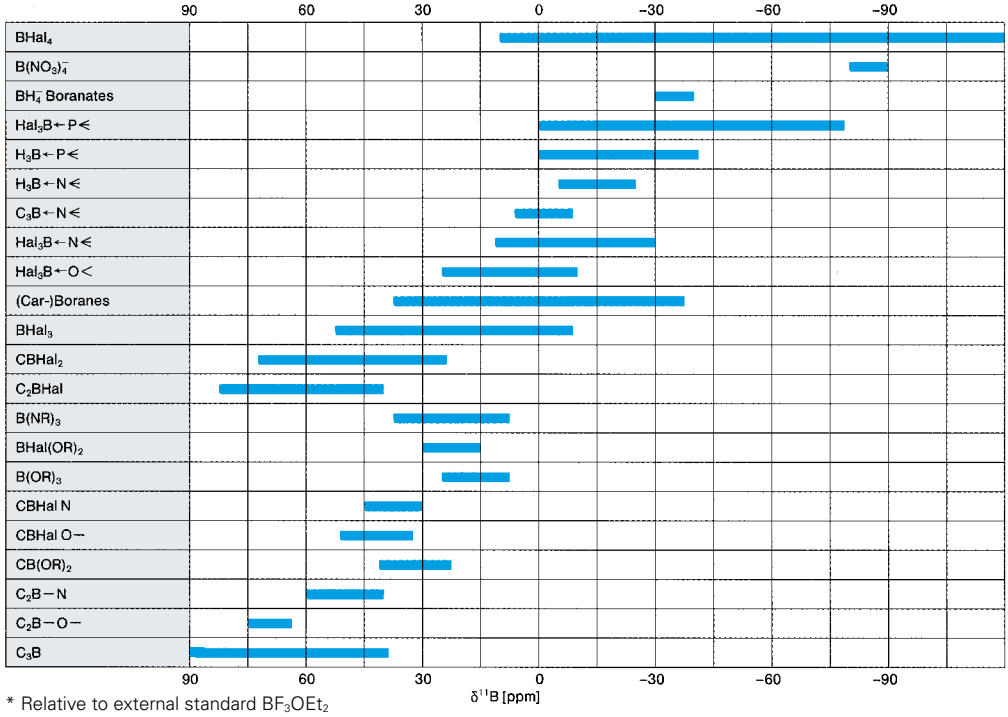
NMR Tables

^{15}N 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.

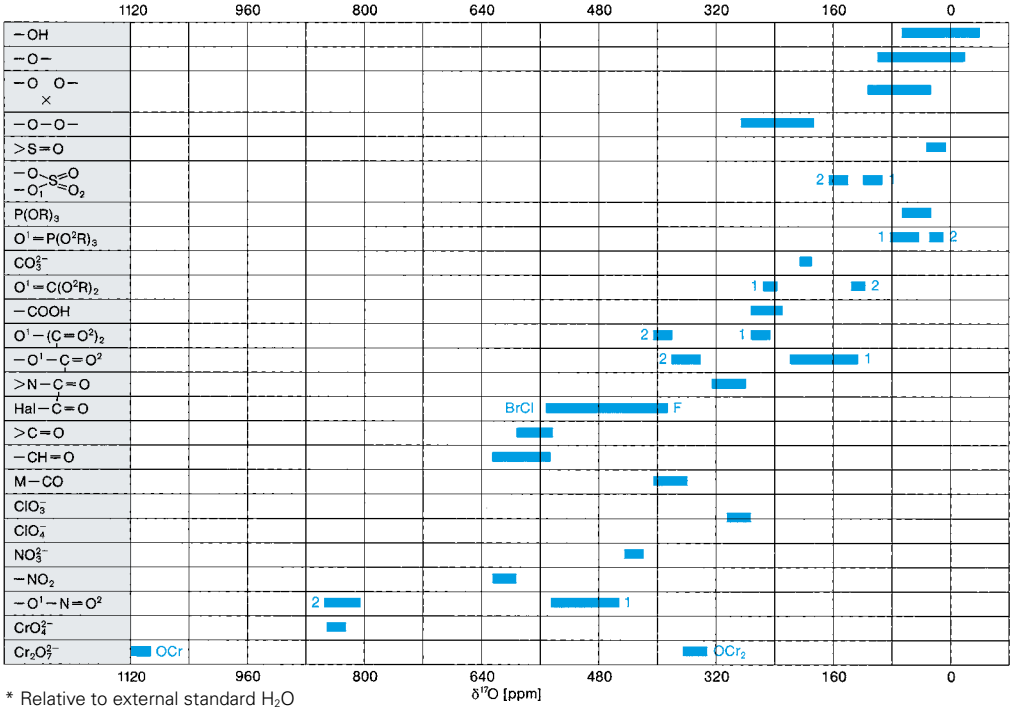
^{11}B Chemical Shifts*



* Relative to external standard BF_3OEt_2

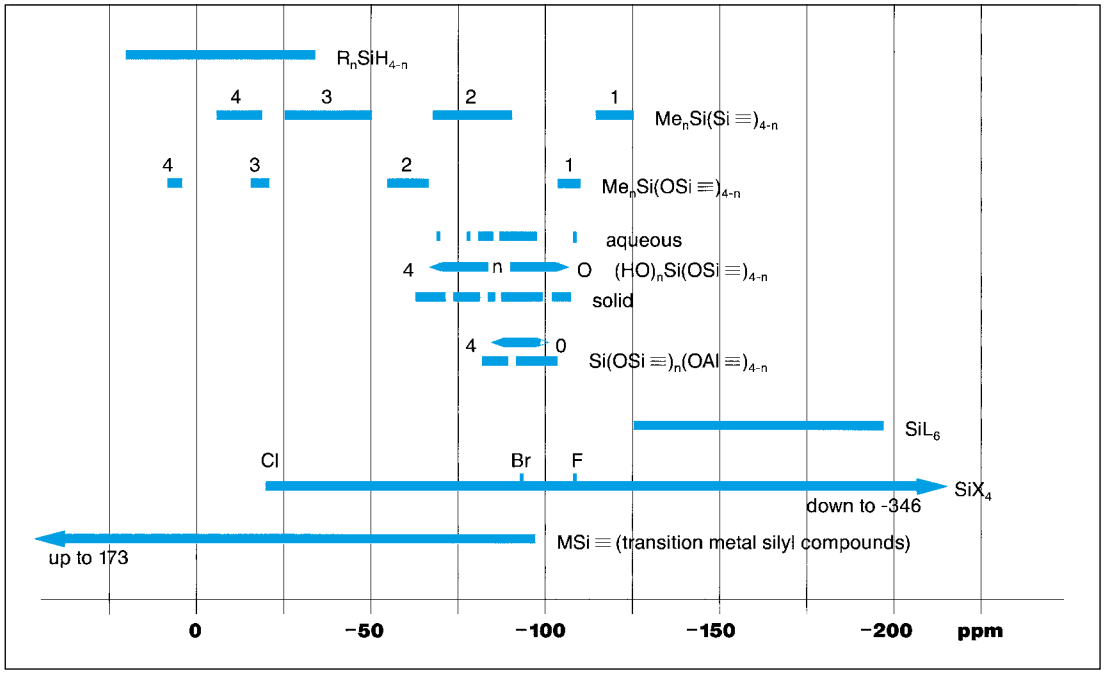
NMR Tables

^{17}O Chemical Shifts*



* Relative to external standard H_2O

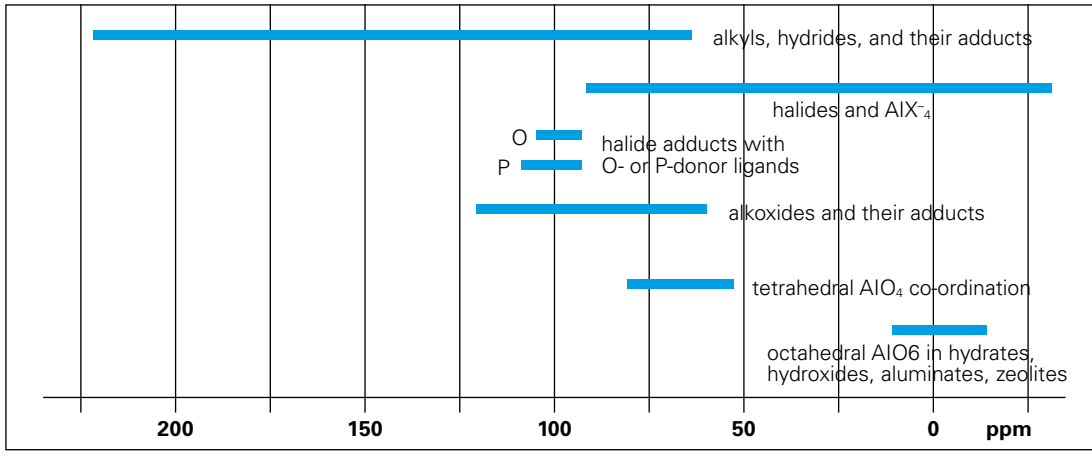
^{29}Si Chemical Shifts*



* Relative to $Si(CH_3)_4$.

NMR Tables

^{27}Al Chemical Shifts*



* Relative to $Al(H_2O)^{3+}_6$.

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	TOF-angio
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-weghted 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	

NMR Tables

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_2CH_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	**–$N(C_6H_5)_2$**	19.3	–4.4	0.6	–5.9
–CH_2Cl	9.1	0.0	0.2	–0.2	**–NO_2**	19.6	–5.3	0.8	6.0
–CH_2Br	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_2OH	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_6H_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_2Br_2	7	$F_2C=CH_2$	-81.3
CF_2H_2	-1436	CFH_2Ph	-207	$F_2C=CF_2$	-135
CF_3R	-60 to -70	CF_2Cl_2	-8	C_6F_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(*n*-Pr)$_3$	-33	$PMeCl_2$	192
P(*i*-Pr)$_3$	-19.4	$PMeBr_2$	184
P(*n*-Bu)$_3$	-32.5	PMe_2F	186
P(*i*-Bu)$_3$	-45.3	PMe_2H	-99
P(*s*-Bu)$_3$	7.9	PMe_2Cl	96.5
P(*t*-Bu)$_3$	63	PMe_2Br	90.5

(b) Phosphorus (V) compounds

	δ / ppm		δ / ppm
Me_3PO	36.2	Me_3PS	59.1
Et_3PO	48.3	Et_3PS	54.5
$[ME_4P]^+$	24.4	$[Et_4P]^+$	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_3PF_2	-158	Me_2PF_3	8.0

NMR Tables

Some Important Silylated Compounds Used as ^{1}H Shift References

Name	Chemical formula	Abbre-viation	Mole-cular weigth	Boiling or melting point (°C)	δ ^{1}H ppm rel. TMS
Tetramethylsilane	$(CH_3)_4Si$	TMS	88.2	BP = 26.3	0
Hexamethyldisilane	$(CH_3)_3Si–Si(CH_3)_3$	HMDS	146.4	BP = 112.3	0.037
Hexamethyldisiloxane	$(CH_3)_3Si–O–Si(CH_3)_3$	HMDSO	162.4	BP = 100	0.055
Hexamethyldisilazane	$(CH_3)_3Si–NH–Si(CH_3)_3$	HMDSA	161.4	BP = 125	0.042
3-(trimethylsilyl)propane sulfonic acid soduim salt 4,4-dimethyl-4-silapentane sodium sulfonate	$(CH_3)_3Si(CH_2)_3SO_3Na$	TSPSA DSS	218.3	MP = 200	0.015
3-(trimethylsilyl)propionic acid sodium salt 4,4-dimethyl-4-silapentane sodium carboxylate	$(CH_3)_3Si(CH_2)_2COONa$	TSP DSC	168.2	MP > 300	0.000
3-(trimethylsilyl) 2,2,3,3-tetra-deuteropropionic acid sodium salt	$(CH_3)_3Si(CD_2)_2COONa$	TSP-d_4	172.2	MP > 300	0.000
Octamethylcyclotetrasiloxane	$(CH_3)_2Si[O–Si(CH_3)_2]_3–O$	OCTS	296.8	BP = 175 MP = 16.8	0.085
1,1,3,3,5,5-hexakis-(trideutero-methyl)-1,3,5-trisilacyclohexane	$(CD_3)_2Si–CH_2–Si(CD_3)_2$ $CH_2–Si(CD_3)_2–CH_2$	CS-d_{18}	216.6	BP = 208	-0.327
Tetrakis-(trimethylsilyl)-methane	$[(CH_3)_3Si]_4C$	TTSM	304.8	MP = 307	0.236

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

Relevant Properties of Cryogenic Fluids

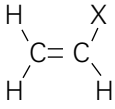
(Liquid helium and nitrogen are used in supercon magnets)

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

NMR Tables

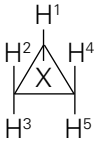
^{1}H, ^{1}H Coupling Constants in Selected Organic Molecules



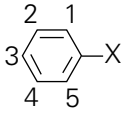
X	$^3J_{cis}$	$^3J_{trans}$	^2J
H	11.6	19.1	2.5
Li	19.3	23.9	7.1
COOH	10.2	17.2	1.7
CN	11.75	17.92	0.91
C_6H_5	11.48	18.59	1.08
CH_3	10.02	16.81	2.08
OCH_3	7.0	14.1	-2.0
Cl	1.3	14.6	-1.4
Br	7.1	15.2	-1.8
F	4.65	12.75	-3.2

$H_3C\text{-}CH_2\text{-}X$

X	^3J
Li	8.90
$Si(C_2H_5)_3$	8.0
H	7.5
C_6H_5	7.62
CN	7.60
I	7.45
Br	7.33
CH_3	7.26
Cl	7.23
$N(C_2H_5)_2$	7.13
OC_2H_5	6.97
$^+O(C_2H_5)_2$	4.7



X	$^3J(1,2)$	$^3J(1,3)$	$^3J(2,4)$	$^3J(3,5)$	$^3J(2,5)$	$^2J(2,3)$
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	$^3J(1,2)$	$^4J(1,3)$	$^5J(1,4)$	$^4J(1,5)$	$^3J(2,3)$	$^4J(2,4)$
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] $^4J(1, CH_3)$ -0.75
$^5J(2, CH_3)$ 0.36
$^6J(3, CH_3)$ -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,j*	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

NMR Tables

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

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

2D	Two-Dimensional
3D	Three-Dimensional
ACCORDION	2D technique, simultaneous incrementing of evolution and mixing times
ADA	**A**lternated **D**elay **A**cquisition
ADC	**A**nalog-to-**D**igital **C**onverter, **A**pparent **D**iffusion **C**onstant
ADEQUATE	**A**stonishingly Sensitive **DoubleE QUA**ntum **T**ransfer **E**xperiment
ADLF	**A**diabatic **D**emagnetization in the **L**aboratory **F**rame
ADRF	**A**diabatic **D**emagnetization in the **R**otating **F**rame
A.E.COSY	**A**lternative **E**xclusive **COSY**
AFP	**A**diabtic **F**ast **P**assage
AHT	**A**verage **H**amiltonian **T**heory
AJCP	**A**diabatic **J** **C**ross **P**olarization
AMCP	**A**mplitude-**M**odulated **C**ross **P**olarization
ANGIO	MR **ANGIO**graphy
APHH-CP	**A**diabatic-**P**assage **H**artmann-**H**ahn **C**ross **P**olarization
APT	**A**ttached **P**roton **T**est
AQ	**A**c**Q**uisition
ARP	**A**diabatic **R**apid **P**assage
ASIS	**A**romatic **S**olvent-**I**nduced **S**hift
ASL	**A**rterial **S**pin **L**abeling
ASTM	**A**merican **S**ociety for **T**esting and **M**aterials
BASE	**BA**sis imaging with **SE**lective-inversion preparation
BB	**B**road**B**and, as in decoupling
BDR	**B**roadband **D**ipolar **R**ecoupling
bEPI	**b**lipped **EPI**
bFFE	**b**alanced **F**ast-**F**ield **E**cho
BIRD	**BI**linear **R**otation **D**ecoupling
BIRD/2	half **BIRD**, bilinear π**/2** pulse
BLEW	A windowless multiple-pulse decoupling sequence
BLEW-*n*	**B**urum-**L**inder-**E**rnst **W**indowless homonuc. dipolar dec. sequence of ***n*** pulses
BMS	**B**ulk **M**agnetic **S**usceptibility
BOLD	**B**lood **O**xygenation **L**evel-**D**ependent contrast (MRI)
BOSS	**B**im**O**dal **S**lice-**S**elective
BP	**BiP**hasic
BPP	**B**loembergen/**P**urcell/**P**ound (theory)
BR-*n*	**B**urum-**R**him homonuclear dipolar decoupling sequence of ***n*** pulses
BSP	**B**loch-**S**iegert **P**hase
BURP	**B**and-selective **U**niform **R**esponse **P**ure-phase pulse
bTFE	**b**alanced **T**urbo **F**ield **E**cho
BW	**B**and**W**idth
BWR	**B**loch-**W**angsness-**R**edfield theory
CA	**C**ontrast **A**gent
CAMELSPIN	**C**ross-relaxation **A**ppropriate for **M**inimolecules **E**mulated by **L**ocked **SPIN**s
CBCA(CO)NH	**C**$\boldsymbol{\beta}$(*i*-1) and **C**$\boldsymbol{\alpha}$(*i*-1), **N**(*i*), H_N(*i*) 3D correl.
CBCANH	**C**$\boldsymbol{\beta}$(*i*,*i*-1) and **C**$\boldsymbol{\alpha}$(*i*,*i*-1), **N**(*i*), H_N(*i*) 3D correl.
CCPPA	**C**oupled **C**luster **P**olarization **P**ropagator **A**pproximation
CE	**C**ontrast-**E**nhanced
CEST	**C**hemical **E**xchange **S**aturation **T**ransfer
CH-COSY	**C**arbon-**H**ydrogen **CO**rrelation **S**pectroscop**Y**
CHESS	**CHE**mical **S**hift **S**elective Imaging Sequence
CHIRP	rf pulse with linear freq. modulation
CIDEP	**C**hemically **I**nduced **D**ynamic **E**lectron **P**olarization
CIDNP	**C**hemically **I**nduced **D**ynamic **N**uclear **P**olarization
CINE	"movie-like" MRI
CISS	**C**onstructive **I**nterference **S**teady **S**tate
CNR	**C**ontrast-to-**N**oise **R**atio
COLOC	**CO**rrelated Spectroscopy via **LO**ng-Range **C**oupling
COLOC-S	**COLOC** with **S**uppression of one-bond correlations
CONOESY	**C**ombined **COSY/NOESY**
CORMA	**CO**mplete **R**elaxation **M**atrix **A**nalysis
CORY-*n*	**CORY** modification of **BR-*n***
COSS	**CO**rrelation with **S**hift **S**caling
COSY	**CO**rrelated **S**pectroscop**Y**
COSY-45	**COSY** with **45°** mixing pulse
COSYDEC	**COSY** with F_1 **DEC**oupling
COSYLR	**COSY** for **L**ong-**R**ange couplings
CP	**C**ross **P**olarization**, C**ircular **P**olarization
CPD	**C**omposite-**P**ulse **D**ecoupling
CPMAS	**C**ross **P**olarization **M**agic-**A**ngle **S**pinning
CPMG	**C**arr-**P**urcell-**M**eiboom-**G**ill Sequence
CRAMPS	**C**ombined **R**otation **A**nd **M**ultiple **P**ulse **S**pectroscopy
CRAZED	**C**orrelated Spectroscopy **R**evamped by **A**symmetric **Z**-gradient **E**cho **D**etection
CRINEPT	**C**ross-correlated **R**elaxation-enhanced **INEPT**
CS	**C**ontiguous **S**lice
CSA	**C**hemical **S**hift **A**nisotropy
CSCM	**C**hemical **S**hift **C**orrelation **M**ap
CSI	**C**hemical **S**hift **I**maging
CT	**C**onstant **T**ime
CW	**C**ontinuous **W**ave
CYCLCROP	**CYCL**ic **CRO**ss **P**olarization
CYCLOPS	**CYCL**ically **O**rdered **P**hase **S**equence
CYCLPOT	**CYCL**ic **PO**larization **T**ransfer
DAC	**D**igital-to-**A**nalog **C**onverter
DAISY	**D**irect **A**ssignment **I**nterconnection **S**pectroscop**Y**
DANTE	**D**elay **A**lternating with **N**utation for **T**ailored **E**xcitation
DAS	**D**ynamic **A**ngle **S**pinning
DCNMR	NMR in Presence of an Electric **D**irect **C**urrent
DD	**D**ipole-**D**ipole
DE	**D**ual **E**cho**,** **D**riven **E**quilibrium

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

DECSY	**D**ouble-quantum **E**cho **C**orrelated **S**pectroscop**Y**
DEFT	**D**riven **E**quilibrium **F**ourier **T**ransform
DEPT	**D**istortionless **E**nhancement by **P**olarization **T**ransfer
DEPTH	spin-echo sequence for spatial localization
DEPTQ	**DEPT** including quaternary carbons
DFT	**D**iscrete **F**ourier **T**ransformation
DICE	**DI**rect **C**onnectivity **E**xperiment
DICOM	**D**igital **I**maging and **CO**mmunications in **M**edicine
DIGGER	**D**iscreet **I**solation from **G**radient-**G**overned **E**limination of **R**esonances
DIPSI	Composite-pulse **D**ecoupling **I**n the **P**resence of **S**calar **I**nteractions
DISCO	**DI**fferences and **S**ums within **CO**SY
DLB	**D**ifferential **L**ine **B**roadening
DNMR	**D**ynamic **NMR**
D.NOESY	**D**irect cross-relaxation **NOESY**
DNP	**D**ynamic **N**uclear **P**olarization
DOC	**D**ouble **CO**nstant-Time sequence
DOPT	**D**ipolar **O**rder **P**olarization **T**ransfer
DOR	**D**ouble-**O**rientation **R**otation
DOSY	**D**iffusion-**O**rdered **S**pectroscop**Y**
DOUBTFUL	**DOUB**le Quantum **T**ransition for **F**inding **U**nresolved **L**ines
DPFGSE	**D**ouble **P**ulsed **F**ield **G**radient **S**pin **E**cho
DQ	**D**ouble **Q**uantum
DQC	**D**ouble **Q**uantum **C**oherence
DQF	**D**ouble **Q**uantum **F**ilter
DQF-COSY	**D**ouble **Q**uantum **F**iltered **COSY**
DQSY	**D**ouble-**Q**uantum CO**SY**
DQ/ZQ	**D**ouble **Q**uantum/**Z**ero **Q**uantum Spectroscopy
DRAMA	**D**ipolar **R**ecovery **A**t the **M**agic **A**ngle
DREAM	**D**ouble-quantum **R**elay **E**nhancement by **A**diabatic **M**ixing
DRESS	**D**epth **RES**olved **S**pectrosocpy
DRIVE	**DRIV**en **E**quilibrium
DRYCLEAN	**D**iffusion-**R**educed water signals in spectroscop**Y** of mole**C**ules moving s**L**ow**E**r th**AN** water
DSA	**D**ata-**S**hift **A**cquisition
DSC	**D**ynamic **S**usceptibility **C**ontrast
DSE	**D**ual **S**pin **E**cho
DTI	**D**iffusion **T**ensor **I**maging
DTRCF	**D**ouble **T**ilted **R**otating **C**oordinate **F**rame
DTSE	**D**ouble **T**urbo **S**pin **E**cho
DUMBO	**D**ecoupling **U**sing **M**ind-**B**oggling **O**ptimization – a numerically optimized phase-modulated homonuc. dipolar dec. sequence
DWI	**D**iffusion-**W**eighted **I**maging
E-BURP	**E**xcitation **BURP** pulse
EC	**E**ddy **C**urrents
E.COSY	**E**xclusive **CO**rrelation **S**pectroscop**Y**
ECO-WURST	**WURST** decoupling with **E**limination of **C**ycling **O**scillations
EFG	**E**lectric **F**ield **G**radient
EM	**E**xponential **M**ultiplication
EMF	**E**lectro**M**agnetic **F**ield **E**lectro**M**otive **F**orce
ENDOR	**E**lectron-**N**uclear **DO**uble **R**esonance
ENMR	**E**lectrophoretic **NMR**
EPI	**E**cho-**P**lanar **I**maging
EPR	**E**lectron **P**aramagnetic **R**esonance
EPS	**E**cho-**P**lanar **S**pectroscopy
ES, ESP	**E**cho **S**pacing
E-SHORT	**E**nhanced **SHORT** repetition MRI
ESR	**E**lectron **S**pin **R**esonace
E.TACSY	**E**xclusive **TACSY**
EXORCYCLE	4-step phase cycle for spin echoes
EXSY	**EX**change **S**pectroscop**Y**
FA	**F**lip **A**ngle
FADE	**FA**SE Acq. with **D**ouble **E**cho
FAIR	**F**low-sensitive **A**lternating **I**nversion **R**ecovery
FASE	**F**ast **A**dvanced **S**pin **E**cho
FAST	**F**ourier-**A**cquired **ST**eady State
FASTMAP	**FAST** B_0 Field **MAP**ping for shimming
FATE	**FA**st **T**urbo **E**cho
FC	**F**low **C**ompensation
FC2D_ANGIO	**F**low-**C**ompensated time-of-flight **2D ANGIO**graphy
FE	**F**ield **E**cho, **F**requency **E**ncoding
FFE	**F**ast **F**ield **E**cho
FFLG	**F**lip-**F**lop **L**ee-**G**oldburg decoupling
FFT	**F**ast **F**ourier **T**ransform
FGRE	**F**ast **G**radient-**R**ecalled **E**cho
FID	**F**ree **I**nduction **D**ecay
FIDS	**FI**tting of **D**oublets and **S**inglets
FieldMap	B_0 **Field Map**ping for localized shimming
FIRFT	**F**ast **I**nversion-**R**ecovery **F**ourier **T**ransform
FISP	**F**ast **I**maging with **S**teady-state **P**recession
FL2D_ANGIO	**FL**ow-sensitive **2D ANGIO**graphy
FLAIR	**FL**uid **A**ttenuation **I**nversion-**R**ecovery
FLASH	**F**ast **L**ow-**A**ngle **SH**ot imaging
FLOCK	Long-range HETCOR using 3 BIRD pulses
FLOPSY	**FI**ip-FI**OP S**pectroscop**Y**
FLOW_MAP	Quantitative **FLOW MAP**ping and PC-angiography
FMP	**F**ast **M**ulti**P**lanar
fMRI	**f**unctional **MRI**
FOCSY	**FO**ldover-**C**orrected **S**pectrospcop**Y**
FONAR	Field-focusing MRI
FOV	**F**ield **O**f **V**iew
FPT	**F**inite **P**erturbation **T**heory
FR	**F**requency **E**ncoding
FS	**F**at **S**aturation, **F**ast **S**can

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

FSE	**F**ast **S**pin **E**cho
FSLG	**F**requency-**S**witched **L**ee-**G**oldburg – a homonuc. dipolar dec. scheme
FSPGR	**F**ast **SP**oiled **GR**adient Echo
FT	**F**ourier **T**ransform
FUCOUP	**FU**lly **COUP**led Spectroscopy
FWHM	**F**ull (line) **W**idth at **H**alf **M**aximum
GARP	**G**lobaly Optimized **A**lternating Phase **R**ectangular **P**ulses
GE	**G**radient **E**cho
GEFC	**G**radient **E**cho with **F**low **C**ompensation
gem-COSY	**gem**inal-filtered **COSY**
GES	**G**radient-**E**cho **S**pectroscopy
GFE	**G**radient **F**ield **E**cho
GRASE	**GRA**dient and **S**pin **E**cho
GRASP	**GR**adient-**A**ccelerated **SP**ectroscopy
GRASS	**G**radient-**R**ecalled **A**cquisition in the **S**teady **S**tate
GRE	**G**radient-**R**ecalled **E**cho
GRECCO	**GR**adient-**E**nhanced **C**arbon **CO**upling
GROESY	**G**radient-Enhanced Selective 1D **ROESY**
GROPE	**G**eneralized compensation for **R**esonance **O**ffset and **P**ulse length **E**rrors
GS	**G**radient **S**pectroscopy
gs- ...	**g**radient-**s**elected ... (e.g. gs-COSY)
H,X-COSY	**H,X** shift correlation (X-detected)
HASTE	**H**alf-Fourier **A**cquisition **S**ingle-shot **T**urbo spin **E**cho
HBHA (CBCA CO) NH	**H**β(i-1) and **H**α(i-1), **N**(i), **H$_N$**(i) 3D correl.
HCACO	**H**α(i), **C**α(i), **C'O**(i) 3D correl.
HCACON	**H**α(i), **C**α(i), **C'O**(i), **N**(i+1) 4D correl.
HCA(CO)N	**H**α(i), **C**α(i), **N**(i+1) 3D correl.
HCA(CO) NNH	**H**α(i), **C**α(i), **N**(i+1), **H$_N$**(i+1) 4D correl.
HCANNH	**H**α(i), **C**α(i), **N**(i), **H$_N$**(i) 3D correl.
(H)CC(CO) NH	**C**α,β,...(i), **N**(i+1), **H$_N$**(i+1) 3D correl.
HCCH-COSY	**H**α(i), **C**α(i), **H**β(i) 3D correl.
HCCH-TOCSY	total correlation of side-chain H and C
HDQC	**H**eteronuclear **D**ouble-**Q**uantum **C**orrelation
HEED	**H**ahn spin-**E**cho **E**xtende**D** sequence
HET2DJ	**HET**eronuclear **2D J**-correlated
HETCOR	**HET**eronuclear **COR**relation Spectroscopy
HETLOC	**HET**eronuclear **LO**ng-range **C**ouplings
HEHAHA	**HE**teronuclear **HA**rtmann **HA**hn
HMBC	**H**eteronuclear **M**ultiple-**B**ond **C**orrelation
HMQ	**H**eteronuclear **M**ultiple-**Q**uantum
HMQC	**H**eteronuclear **M**ultiple-**Q**uantum **C**oherence
HMSC	**H**eteronuclear **M**ultiple- and **S**ingle-bond **C**orrelation
HNCA	**H$_N$**(i), **N**(i), **C**α(i) and **C**α(i-1) 3D shift correlation
HNCA-J	3D **HNCA** to measure $^3J(H_N,H\alpha)$
HN(CA)NNH	**H$_N$**(i), **N**(i), **N**(i+1) and **N**(i-1) 3D correl.
HN(CA)CO	**H$_N$**(i), **N**(i), **C'O**(i), and **C'O**(i-1) 3D shift correlation
H(N)CACO	**H$_N$**(i), **C**α(i), **C'O**(i) 3D shift correlation
HNCAHA	**H$_N$**(i), **N**(i), **C**α(i), **H**α(i) 4D shift correlation
HNCO	**H$_N$**(i), **N**(i), **C'O**(i-1) 3D shift correlation
HN(CO)CA	**H$_N$**(i), **N**(i), **C**α(i-1) 3D shift correlation
H(N)COCA	**H$_N$**(i+1), **C'O**(i), **C**α(i) 3D shift correlation
HN(CO) CAHA	**H$_N$**(i+1), **N**(i+1), **C**α(i), **H**α(i) 4D shift correlation
HOESY	**H**eteronuclear **O**verhauser **E**ffect **S**pectroscop**Y**
HOHAHA	**HO**monuclear **HA**rtmann-**HA**hn Spectroscopy
HORROR	double-quantum **HO**mo-nuclea**R RO**tary **R**esonance
HQQC	**H**eteronuclear **Q**uadruple-**Q**uantum **C**orrelation
HR	**H**igh **R**esolution
HRPA	**H**igher **R**andom **P**hase **A**pproximation
HS	**H**omo**S**poil
HSL	**H**eteronuclear **S**pin **L**ock
HSQC	**H**eteronuclear **S**ingle-**Q**uantum **C**oherence
HTQC	**H**eteronuclear **T**riple-**Q**uantum **C**orrelation
I-BURP	**I**nversion **BURP** pulse
ICE	**I**ndirect **C**onnectivity **E**xperiment
IDESS	**I**mproved **DE**pth **S**elective single surface coil **S**pectroscopy
IDR	**I**nverted **D**irect **R**esponse
IEPI	**I**nterleaved **EPI**
IFT	**I**nverse **FT**
IGLO	**I**ndividual **G**auge for different **L**ocalized **O**rbitals
INADE-QUATE	**I**ncredible **N**atural **A**bu-dance **DoublE QUA**natum **T**ransfer **E**xperiment
INAPT	**INEPT** with selective 1H excitation
INDOR	**IN**ternuclear **DO**uble **R**esonance
INEPT	**I**nsensitive **N**uclei **E**nhanced by **P**olarization **T**ransfer
INEPT+	**INEPT** with refocusing period for in-phase multiplets
INEPT-R	**INEPT R**efocused for 1H-dec. spectra
INSIPID	**IN**adequate **S**ensitivity **I**mprovement by **P**roton **I**ndirect **D**etection
IntraGate-FLASH	Cardiac and respiration cine MRI with retrospective (trigger-free) gating
INVERSE	H, X correlation via ^{1}H detection
IPAP	**I**n-**P**hase **A**nti-**P**hase (in 2D)
IR	**I**nversion-**R**ecovery
IRMA	**I**terative **R**elaxation **M**atrix **A**nalysis
ISECR	**I**n-pha**SE CR**oss peaks (method)

Abbreviations and Acronyms Used in Magnetic Resonance

ISIS	**I**mage-**S**elected **I**n-vivo **S**pectroscopy (single-voxel)
IST	**I**rreducible **S**pherical **T**ensor
IVIM	**I**ntra**V**oxel **I**ncoherent **M**otion
JCP	**J C**ross-**P**olarization
J-mod	**J mod**ulation
JR	**J**ump-and-**R**eturn sequence (90_y-τ-90_{-y})
J-res	**J-res**olved 2D
LAS	**L**aboratory **A**xis **S**ystem
LASE	**L**ow-**A**ngle **SE**
LB	**L**ine **B**roadening (via EM)
LG	**L**orentz-**G**auss window function
LIS	**L**anthanide **I**nduced **S**hift
LORG	**L**ocal **OR**i**G**in
LOSY	**LO**calized **S**pectroscop**Y**
LP	**L**inear **P**olarization, **L**inear **P**rediction
LPSVD	**L**inear **P**rediction using **S**ingular **V**alue **D**ecomposition
LSR	**L**anthanide **S**hift **R**eagent
LUT	**L**ook**U**p **T**able
MAGROFI	**MA**gnetization **G**rid **RO**tating-**F**rame **I**maging
MARCO POLO	**M**ultiple **A**nalysis by **R**eduction of **C**ross peaks and **O**rdering of **P**atterns in an **O**verdetermined **L**ibrary **O**rganization
MARDI-GRAS	**M**atrix **A**nalysis of **R**elaxati-on for **DI**stance **G**eomet**R**y of an **A**queous **S**tructure
MARF	**M**agic **A**ngle in the **R**otating **F**rame
MAS	**M**agic-**A**ngle **S**pinning
MASS	**M**agic-**A**ngle **S**ample **S**pinning
MAST	**M**otion **A**rtifact **S**uppression **T**echnique
MDEFT	**M**odified **D**riven **E**quilibrium **FT** method
ME	**M**ulti**E**cho
MEDUSA	Technique for the Determination of Dynamic Structures
MEM	**M**aximum **E**ntropy **M**ethod
MEMP	**M**ulti**E**cho **M**ulti**P**lanar
MESS	**M**ulti**E**cho **S**ingle **S**hot
MFISP	**M**irrored **FISP** (PSIF)
MGE	**M**ultiple **G**radient **E**cho
MININIP	**MIN**inmum **I**ntensity **P**rojection
MIP	**M**aximum **I**ntensity **P**rojection
MLEV	M. Levitt's CPD sequence
MLM	**M**aximum **L**ikelihood **M**ethod
MOTSA	**M**ultiple **O**verlapping **T**hin **S**lab(Slice) **A**cquisition
MP	**M**ultiple **P**ulse, **M**ulti**P**lanar, **M**agnetization-**P**repared
MPF*n*	**M**ultiple-Pulse Decoupling with **P**hase and **F**requency Switching with ***n*** offsets
MP-GR	**M**ulti**P**lanar **G**radient-**R**e-called Acq. in Steady State
MPR	**M**ulti**P**lanar **R**econstruction
MP-RAGE	**M**agnetization-**P**repared **RA**pid **G**radient **E**cho (MP-GRE)
MQ	**M**ultiple-**Q**uantum
MQC	**M**ultiple-**Q**uantum **C**oherence
MQF	**M**ultiple-**Q**uantum **F**ilter
MQHPT	**M**ultiple-**Q**uantum **H**eteronuclear **P**olarization **T**ransfer
MQS	**M**ultiple-**Q**uantum **S**pectroscopy
MR	**M**agnetic **R**esonance
MRA	**MR A**ngiography
MREV-*n*	**M**ansfield-**R**him-**E**lleman-**V**aughan homonuc. dipolar dec. cycle of ***n*** pulses
MRV	**MR V**enography
MRI	**M**agnetic **R**esonance **I**maging
MRS	**M**agnetic **R**esonance **S**pectroscopy
MRSI	**M**agnetic **R**esonance **S**pectroscopic **I**maging
MRT	**M**agnetic **R**esonance **T**omography
MS	**M**ulti**S**lice
mSENSE	**m**odified **SENSE**
MS-EPI	**M**ulti**S**hot **EPI**
MSHOT-*n*	**M**agic **S**andwich **H**igh-**O**rder **T**runcation homo-nuc. dipolar decoupling sequence with ***n*** TREV-4 sandwiches
MSME	**M**ulti**S**lice **M**ulti**E**cho (T2 mapping)
MSOFT	**M**ulti**S**lice **O**ff-resonance **FaT** Suppression
MSP	**M**ultiple **S**ensitive **P**oint
MSPGSE	**M**ultiple-**S**tepped **PGSE**
MT	**M**agnetization **T**ransfer
MTC	**M**agnetization **T**ransfer **C**ontrast
MTSA	**M**ultiple **T**hin-**S**lab **A**cquisition
MUSIC	**MU**ltiplicity-**S**elective **I**n-phase **C**oherence transfer
MVS	**M**ultiple **V**olume **S**pectroscopy
NEDOR	**N**uclear **E**lectronic **DO**uble **R**esonance
NERO	**N**onlinear **E**xcitation with **R**ejection on **R**esonance
NEWS	**N**arrow-gap non-**E**xcitation for **W**ater **S**uppression
NEX	**N**umber of **EX**citations
NMR	**N**uclear **M**agnetic **R**esonance
NOE	**N**uclear **O**verhauser **E**ffect
NOE-DIFF	**NOE-DIFF**erence spectroscopy
NOESY	**NOE**-based 2D shift correlation
NOVEL	**N**uclear **O**rientation **V**ia **E**lectron spin **L**ocking
NPW	**N**o **P**hase **W**rap
NQCC	**N**uclear **Q**uadrupole **C**oupling **C**onstant
NQR	**N**uclear **Q**uadrupole **R**esonance
NQS	**N**on-**Q**uaternary **S**uppression
NSPECT	**N**on-localized **SPECT**roscopy
OBTUSE	**O**ffset **B**inomial **T**ailored for **U**niform **S**pectral **E**xcitation
OCS	**O**ptimized **C**osine-**S**ine pulse
ODMR	**O**ptically **D**etected **M**agnetic **R**esonance
OS	**O**vercontiguous **S**lices
OSIRIS	**O**uter-Volume-**S**uppressed **I**mage-**R**elated **I**n vivo **S**pectroscopy – a modifica-tion of ISIS
PACE	**P**rospective **A**cquisition **C**orr**E**ction
PAR	**P**hase-**A**lternated **R**otation of magnetization

Abbreviations and Acronyms Used in Magnetic Resonance

PARACEST	**PARA**magnetic **C**hemical **E**xchange **S**aturation **T**ransfer
PAS	**P**rincipal **A**xis **S**ystem
PC	**P**hase **C**ontrast
PCA	**P**hase **C**ontrast **A**ngio-graphy
P.COSY	**P**urged **COSY**
PD	**P**roton **D**ensity
PDLF	**P**roton-**D**etected **L**ocal **F**ield
PE	**P**hase **E**ncoding
P.E.COSY	**P**rimitive **E.COSY**, **P**urged **E**xclusive **COSY**
PEDRI	**P**roton-**E**lectron **D**ouble **R**esonance **I**maging
PELF	**P**roton-**E**ncoded **L**ocal **F**ield
PENDANT	**P**olarization **EN**hancement **D**uring **A**ttached **N**ucleus **T**esting
PEP	**P**reservation of **E**quivalent **P**athways
PFG	**P**ulsed **F**ield **G**radient
PFGSE	**P**ulsed **F**ield **G**radient **S**pin **E**cho
PGSE	**P**ulsed **G**radient **S**pin **E**cho
PISEMA	**P**olarization **I**nversion with **S**pin **E**xchange at the **M**agic **A**ngle
PITANSEMA	**P**olarization **I**nversion **T**ime **A**veraged **N**utation **S**pin **E**xchange at the **M**agic **A**ngle
PJR	**P**ower-adapted **J**ump and **R**eturn
PMFG	**P**ulsed **M**agnetic **F**ield **G**radient
PMLG	**P**hase-**M**odulated **L**ee-**G**oldburg dipolar decoupling
PMRFI	**P**hase-**M**odulated **R**otating-**F**rame **I**maging
POF	**P**roduct **O**perator **F**ormalism
POMMIE	**P**hase **O**scillations to **M**axi**MI**ze **E**diting
POST	**P**ermutationally **O**ffset-**ST**abilized
PRE	**P**roton **R**elaxation **E**nhancement
Presat	**Presat**uration (usually of solvent)
PRESS	**P**oint-**RES**olved **S**pectroscopy
PRFT	**P**artially **R**elaxed **F**ourier **T**ransform
PROPELLER	**P**eriodically **R**otated **O**ver-lapping **P**aral**lEL** **L**ines with **E**nhanced **R**econstruction
PS	**P**artial **S**aturation
PS-COSY	**P**hase-**S**ensitive **COSY**
PSD	**P**hase-**S**ensitive **D**etection
PSIF	mirrored **FISP** (SE acquisition)
PT	**P**olarization **T**ransfer
PW	**P**ulse **W**idth
PWI	**P**erfusion-**W**eighted **I**maging
Q	**Q**uality **F**actor (of RF coil/circuit) **Q**uantitative … (e.g. **QMRI**, **QCSI**)
Q.F	**Q**uadrupole moment/**F**ield gradient (interaction or relaxation mechanism)
Q Flow	**Flow Q**uantification
QPD	**Q**uadrature **P**hase **D**etection
QUEST	**QU**ick **E**cho **S**plit Imaging **T**echnique
QUIPSS	**QU**antitative **I**maging of **P**erfusion using a **S**ingle **S**ubtraction
RAM	**R**apid **A**cquisition **M**atrix
RARE	**R**apid **A**cquisition **R**elaxation **E**nhanced
RAREst	**RARE** with **s**hort **t**E using slew-rate-optimized gradients
RAREVTR	**RARE** with **V**ariable **TR** (simultaneous T_1 & T_2 mapping)
RASE	**R**apid **A**cquisition **S**pin **E**cho
RBW	**R**eceiver **B**and**W**idth
RCF	**R**otating **C**oordinate **F**rame
RCT	**R**elayed **C**oherence **T**ransfer
RE	**R**apid **E**xcitation (MRI)
REAPDOR	**R**otational **E**cho **A**diabatic **P**assage **DO**uble **R**esonance
RE-BURP	**Re**focused **B**and-selective **U**niform **R**esponse **P**ure phase
RECSY	Multistep **RE**layed **C**oherence **S**pectroscop**Y**
REDOR	**R**otational **E**cho **DO**uble **R**esonance
RELAY	**RELAY**ed Correlation Spectroscopy
REPAY	**R**everse **E**diting of **P**rotons **A**ccording to multiplicit**Y**
REREDOR	**R**otor-**E**ncoded **REDOR**
REST	**RE**gional **S**aturation **T**echnique
RF	**R**adio **F**requency
RFDR	**RF-D**riven **R**ecoupling
RF-FAST	**RF**-spoiled **FAST**
RFOV	**R**ectangular **FOV**
RICE	**R**apid **I**maging using **C**om-posite **E**cho
RIDE	**RI**ng **D**own **E**limination
RINEPT	**R**everse **INEPT**
RISE	**R**apid **I**maging using **S**pin **E**cho
RMSD	**R**oot-**M**ean-**S**quare **D**eviation
ROAST	**R**esonant **O**ffset **A**veraging in the **ST**eady State
RODI	**RO**tatin-grame relaxation **D**ispersion **I**maging
ROE	**R**otating-frame **O**verhauser **E**ffect
ROESY	**ROE**-based 2D shift correlation
ROI	**R**egion **O**f **I**nterest
ROPE	**R**espiratory **O**rdered **PE**
ROTO	**RO**ESY-**TO**CSY Relay
RPA	**R**andom **P**hase **A**pproximation
RR	**R**otational **R**esonance
RSSARGE	**R**F-**S**poiled **SARGE**
RT	**R**espiratory **T**rigger
RUFIS	**R**otating **U**ltra**F**ast **I**maging **S**equence
SA	**S**hielding **A**nisotropy
SAR	**S**pecific **A**bsorption **R**ate (RF)
SARGE	**S**poiled steady-state **A**cquisition with **R**ewinded **G**radient **E**cho
SAT	**SAT**uration
SB	**S**ine-**B**ell window function
SC	**S**calar **C**oupling
S.COSY	**COSY** with shift **S**caling in F1
SCT	**SC**an **T**ime
SCUBA	**S**timulate **C**ross peaks **U**nder **B**leached **A**lphas
SD	**S**pin **D**ipolar

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

SDDS	**S**pin **D**ecoupling **D**ifference **S**pectroscopy
SDEPT	**S**elective **DEPT**
SE	**S**pin **E**cho
SECSY	**S**pin-**E**cho **C**orrelated Spectroscop**Y**
SEDOR	**S**pin-**E**cho **DO**uble **R**esonance
SEDRA	**S**imple **E**xcitation for **D**ephasing of **R**otational echo **A**mplitudes
SEDUCE	**SE**lective **D**ecoupling **U**sing **C**rafted **E**xcitation
SEFT	**S**pin-**E**cho **F**ourier **T**ransform Spectroscopy (with J modulation)
SELCOSY	**SEL**ective **COSY**
SELTICS	**S**ideband **EL**imination by **T**emporary **I**nterruption of the **C**hemical **S**hift
SELINCOR	**SEL**ective **IN**verse **COR**relation
SELINQUATE	**SEL**ective **IN**ADE**QUATE**
SELRESOLV	**SEL**ective **RES**olution of C,H Coupling
SEMS	**S**pin-**E**cho **M**ulti**S**lice
SEMUT	**S**ubspectral **E**diting Using a **MU**ltiple-Quantum **T**rap
SENSE	**SENS**itivity **E**ncoding
sEPI	**s**piral **EPI**
SEPT	**S**elective IN**EPT**
SERF	**SE**lective **R**e**F**ocussing
SESAM	**SE**mi-**S**elective **A**cquisition **M**odulated (Decoupling)
SFAM	**S**imultaneous **F**req. and **A**mpl. **M**odulation
SFORD	**S**ingle **F**requency **O**ff-**R**esonance **D**ecoupling
SGSE	**S**teady-**G**radient **S**pin-**E**cho
SHECOR	**S**elective **HE**teronuclear **COR**relation
SHORT	**SHORT** repetition techniques
SI	**S**pectroscopic **I**maging
SIAM	**Si**multaneous acq. of **I**n-phase and **A**ntiphase **M**ultiplets
SIP	**S**aturation **I**nversion **P**rojection
SIMBA	**S**elective **I**nverse **M**ultiple-**B**ond **A**nalysis
SINEPT	**SINE**-dependent **PT**
SINGLE PULSE	**SINGLE PULSE**-acquire spectroscopy
SIS	**S**ubstituent-**I**nduced **S**hift
SJR	**S**econd-order **J**ump and **R**eturn
SKEWSY	**SKEW**ed Exchange Spectroscop**Y**
SL	**S**pin-**L**ock pulse
SLF	**S**eparated **L**ocal **F**ield
SLITDRESS	**SLI**ce in**T**erleaved **D**epth **RE**solved **S**urface coil **S**pectroscopy
SLOPT	**S**pin-**LO**cking **P**olarization **T**ransfer
SMART	**S**himadzu **M**otion **A**rtifact **R**eduction **T**echnique
SMASH	**S**hort **M**inimum **A**ngle **SH**ot, **S**i**M**ultaneous **A**cquisition of **S**patial **H**armonics
SNR or S/N	**S**ignal-to-**N**oise **R**atio
SOPPA	**S**econd-**O**rder **P**olarization **P**ropagator **A**pproach
SORS/STC	**S**lice-selective **O**ff-**R**esonance **S**inc Pulse **/ S**aturation **T**ransfer **C**ontrast
SPACE	**SPA**tial and **C**hemical-Shift Encoded **E**xcitation
SPAIR	**SP**ectral Selection **A**ttenuated **I**nversion **R**ecovery
SPECIFIC-CP	**SPEC**trally **I**nduced **F**iltering **I**n **C**ombination with **C**ross **P**olarization
SPEED	**S**wap **P**has**E**-**E**ncoded **D**ata
SPGR	**SP**oiled **G**radient-**R**ecalled
SPI	**S**elective **P**opulation **I**nversion
SPIDER	**S**teady-state **P**rojection **I**maging with **D**ynamic **E**cho **T**rain **R**eadout
SPIO	**S**uper**P**aramagnetic **I**ron **O**xide
SPIR	**S**pectral **P**resaturation **I**nversion-**R**ecovery
SPIRAL	MRI with **SPIRAL** *k*-space scan
SPRITE	**S**ingle-**P**oint **R**amped **I**maging with **T**1 **E**nhancement
SPT	**S**elective **P**opulation **T**ransfer
SQ	**S**ingle-**Q**uantum
SQC	**S**ingle-**Q**uantum **C**oherence
SQF	**S**ingle-**Q**uantum **F**ilter
SR	**S**aturation-**R**ecovery
SRP	**S**elf-**R**efocusing **P**ulse
SS	**S**lice **S**election (gradient), **S**ingle **S**lice
SSB	**S**hifted **S**ine-**B**ell window function
SSFP	**S**teady-**S**tate **F**ree **P**recession
SSFSE	**S**ingle-**S**hot **FSE**
SSI	**S**olid **S**tate **I**maging
SSMP	**S**ingle-**S**lice **M**ultiple-**P**hase
ssNMR	**s**olid-**s**tate **NMR**
SSTSE/T2	**S**ingle-**S**hot **TSE** with **T2** weighting
ST	**S**aturation **T**ransfer, **S**lice **T**hickness
STAGE	**S**mall **T**ip **A**ngle **GE**
STE	**ST**imulated **E**cho
STEAM	**ST**imulated **E**cho **A**cquisition **M**ode for imaging
STEP	**STE P**rogressive Imaging
STERF	**S**teady-State **TE**chnique with **R**efocused **F**ID
STIR	**S**hort **T**1 **I**nversion-**R**ecovery
STREAM	**S**uppressed **T**issue with **RE**freshment **A**ngiography **M**ethod
STUD	**S**ech/**T**anh **U**niversal **D**ecoupling – an adiabatic decoupling scheme
SUBMERGE	**SU**ppression **B**y **M**istuned **E**cho and **R**epetitive **G**radient **E**pisodes
SUSAN	**S**pin decoupling employing **U**ltra-broadband inversion sequences generated via **S**imulated **AN**nealing
SWATTR	**S**elective **W**ater **A**ttenuation by **T2** and **T1 R**elaxation
SVS	**S**ingle-**V**olume **S**pectroscopy
T1 ...	**T1**-weighted ... (method)
T1W	**T1-W**eighted
T2 ...	**T2**-weighted ... (method)
T2W	**T2-W**eighted
T2*W	**T2*-W**eighted
TACSY	**TA**ylored **C**orrelation Spectroscop**Y**
TANGO	**T**esting for **A**djacent **N**uclei with a **G**yration **O**perator

NMR Tables

Abbreviations and Acronyms Used in Magnetic Resonance

TART	**T**ip **A**ngle **R**educed T_1 Imaging
TD	**T**rigger **D**elay, **T**ime **D**ifference
TCF	**T**ime **C**orrelation **F**unction
TE	**T**ime delay between excitation and **E**cho maximum
TEDOR	**T**ransferred-**E**cho **DO**uble **R**esonance
TEI	**TE** **I**nterleaved
TF	**T**urbo **F**actor
TFE	**T**urbo **F**ield **E**cho
TGSE	**T**urbo **G**radient **S**pin **E**cho
THRIVE	**T**1W **H**igh-**R**esolution **I**sotropic **V**olume **E**xamination
TI	**T**ime following **I**nversion
TIR	**T**urbo **IR**
TMR	**T**opical **M**agnetic **R**esonance
TOBSY	**TO**tal through-**B**ond correlation **S**pectroscop**Y**
TOCSY	**TO**tal **C**orrelation **S**pectroscop**Y**
TOF	**T**ime-**O**f-**F**light
TOE	**T**runcated N**OE**
TONE	**T**ilt-**O**ptimized **N**onsaturated **E**xcitation
TORO	**TO**CSY-**RO**ESY Relay
TOSS	**TO**tal **S**uppression of **S**idebands
TPPI	**T**ime-**P**roportional **P**hase **I**ncrementation
TPPM	**T**wo-**P**ulse **P**hase **M**odulation
TPR	**T**ime and **P**hase **R**eversal
TQ	**T**riple-**Q**uantum
TQF	**T**riple-**Q**uantum **F**ilter
TR	**T**ime for **R**epetition of excitation
T/R	**T**ransmit/**R**eceive
TRAPDOR	**TRA**nsfer of **P**opulations in **DO**uble **R**esonance
TRCF	**T**ilted **R**otating **C**oordinate **F**rame
TREV-*n*	**T**ime-**REV**ersal echo sequence of ***n*** pulses for homonuc. dipolar dec.
TRNOE	**TR**ansferred **NOE**
TROSY	**T**ransverse **R**elaxation **O**ptimized **S**pectroscop**Y**
T-ROESY	**T**ransverse **ROESY**

TrueFISP	**FISP** with balanced gradient waveform
TS	**T**ime of **S**aturation
TSE	**T**urbo **S**pin **E**cho
TSETSE	double-resonance **T**wo-**S**pin **E**ffect for correlation spectroscopy
TSR	**T**otal **SR**
Turbo-FLASH	**FLASH** sequence during one IR period
U-BURP	**U**niversal **BURP** pulse
UE	**U**npaired **E**lectron (relaxation mechanism)
UFSE	**U**ltra**F**ast **SE**
UNCOSY	**UN**iform excitation **COSY**
USPIO	**U**ltra**S**mall **P**aramagnetic **I**ron **O**xide
UTE	**U**ltra-short **TE** radial scan
UTSE	**U**ltra-short **TSE**
VAPRO	**VA**riable **PRO**jection method
VAS	**V**ariable **A**ngle **S**pinning
VE	**V**elocity-**E**ncoded
VEC	**V**elocity-**E**ncoded **C**ine (MRI)
VEMP	**V**ariable-**E**cho **M**ulti**P**lanar
VENC	**V**elocity **ENC**oding value
VEST	**V**olume **E**xcitation **ST**imulated echoes
VIGRE	**V**olumetric **I**nterpolated **GR**adient **E**cho
VOI	**V**olume **O**f **I**nterest
VOSING	**VO**lume-selective **S**pectral edit**ING**
VOSY	**VO**lume-Selective **S**pectroscop**Y**
VPS	**V**olumes **P**er **S**egment
VSOP	**V**ery **S**mall superparamagnetic iron **O**xide **P**articles
WAHUHA	**WA**ugh-**HU**ber-**HA**eberlen Sequence
WALTZ	CPD Sequence Containing the Elements 1-2-3
WATER-GATE	**WATER** suppression through **GrA**dient **T**ailored **E**xcitation
WATR	**W**ater **A**ttenuation by **T**ransverse **R**elaxation
WEFT	**W**ater **E**liminated **F**ourier **T**ransform
WET	**W**ater suppression **E**nhanced through **T**1 effects

WFOP	**W**ater **F**at **O**pposed **P**hase
WFS	**W**ater **F**at **S**eparation (Shift Difference)
WHH-*n*	**WAHUHA** dec. cycle of ***n*** pulses
WIM-*n*	**W**indowless **I**sotropic **M**ixing dec. cycle of ***n*** pulses
WURST	**W**ideband, **U**niform **R**ate, and **S**mooth **T**runcation – an adiabatic decoupling sequence
XCORFE	H, **X** **COR**relation using a **F**ixed **E**volution time
XD-NOESY	e**X**change-**D**ecoupled **NOESY**
X-FILTER	Selection of ^{1}H-^{1}H correlation when both H are coupled to X
X-HALF-FILTER	Selection of ^{1}H-^{1}H correlation when one H is coupled to X
Z-COSY	**Z**-filtered **COSY**
Z-FILTER	pulse sandwich for elimination of signal components with dispersive phase
ZECSY	**Z**ero-Quantum-**E**cho **C**orrelation **S**pectroscop**Y**
ZIP	**Z**ero-fill **I**nterpolation **P**rocessing
ZQ	**Z**ero **Q**uantum
ZQC	**Z**ero-**Q**uantum **C**oherence
ZQF	**Z**ero-**Q**uantum **F**ilter
ZZ-Spectroscopy	Selection of coherences involving ZZ or longitudinal two-spin order
ZZZ-Spectroscopy	Selection of coherences involving longitudinal 3-spin order
β-COSY	COSY with low-angle mixing pulse
Ψ-COSY	pseudo-COSY using incremented freq.-selective excitation

NMR Tables

Symbols for NMR and Related Quantities*

Roman alphabet	
a or A	Hyperfine (electron-nucleus) coupling constant
$A_q^{(l,m)}$	The mth component of an irreducible tensor of order l representing the nuclear spin operator for an interaction of type q
$\boldsymbol{B}$	Magnetic field (strictly the magnetic flux density or magnetic induction)
$\boldsymbol{B}_0$	Static magnetic field of an NMR spectrometer
$\boldsymbol{B}_1$, $\boldsymbol{B}_2$	Radiofrequency magnetic fields associated with frequencies ν_1, ν_2
$\boldsymbol{B}_L$	Local magnetic field of random field or dipolar origin
$\boldsymbol{C}$	Spin-rotation interaction tensor
C_X	Spin-rotation coupling constant of nuclide X
$\boldsymbol{D}$	Dipolar interaction tensor
$D_{i,j}$	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 ^{1}H
$\boldsymbol{E}$	Electric field strength
F	Spectral width
F_1, F_2 or f_1, f_2	The two frequency dimensions of a two-dimensional spectrum
$\hat{\boldsymbol{F}}_G$	Nuclear spin operator for a group, G, of nuclei
F_G	Magnetic quantum number associated with $\hat{\boldsymbol{F}}_G$
g	Nuclear or electronic g factor (Landé splitting factor)
G	Magnetic field gradient amplitude
$\hat{\boldsymbol{H}}$	Hamiltonian operator
$H_{i,j}$	Matrix element of Hamiltonian operator
$\hat{\boldsymbol{I}}_j$	Nuclear spin operator for nucleus j
$\hat{I}_{j+}$, $\hat{I}_{j-}$	'Raising' and 'lowering' spin operators for nucleus j
I_j	Magnetidc quantum number associated with $\hat{\boldsymbol{I}}_j$
$\boldsymbol{J}$	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}

$\boldsymbol{L}$	Angular momentum
m_j	Eigenvalue of $\hat{\boldsymbol{I}}_{jz}$ (magnetic component quantum number)
m_{tot}	Total magnetic component quantum number for a spin system (eigenvalue of $\sum_j \hat{\boldsymbol{I}}_{jz}$)
$m_{tot}(X)$	Total magnetic component quantum number for X-type nuclei
$\boldsymbol{M}_0$	Equilibrium macroscopic magnetization per unit volume in the presence of $\boldsymbol{B}_0$
M_x, M_y, M_z	Components of macroscopic magnetization per volume
M_n	nth 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
$\boldsymbol{q}$	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
$R_{1\rho}^X$	Longitudinal relaxation rate constant for nucleus X in the reference frame rotating with $\boldsymbol{B}_1$
S	Signal intensity
$\hat{\boldsymbol{S}}$	Electron (or, occasionally, nuclear) spin operator; cf. $\hat{\boldsymbol{I}}$
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
$T_{1\rho}^X$	Longitudinal relaxation time for the X nucleus in the reference frame rotating with $\boldsymbol{B}_1$
T_d	Pulse (recycle) delay
T_{ac}	Acquisition time
$T_q^{(l,m)}$	The mth 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)*

NMR Tables

Symbols for NMR and Related Quantities*

$\boldsymbol{V}$	Electric field gradient tensor. $\boldsymbol{V} = e\boldsymbol{q}$, where e is the elementary charge
$V_{\alpha\beta}$	Elements of Cartesian electric field gradient tensor
W_0, W_1, W_2	Relaxation rate constants (transition probabilities per time) between energy levels differing by 0, 1 and 2 in m_{tot}
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-½ 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-½ 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 ($\Delta\chi = \chi_{\parallel} - \chi_{\perp}$); (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 $\boldsymbol{B}_0$
$\boldsymbol{\mu}$	(i) Magnetic dipole moment (component μ_z along $\boldsymbol{B}_0$); (ii) electric dipole moment
μ_0	Permeability of the vacuum
μ_B	Bohr magneton (earlier β_e)
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)
Ξ_X	Normalized resonance frequency for nucleus X relative to ν_H for tetramethylsilane (TMS) at the same $\boldsymbol{B}_0$ field; $\Xi_x = 100\ \nu_x/\nu_H$ (TMS)
ρ	Density matrix
$\hat{\rho}$	Density operator
ρ_{ij}	Element of matrix representation of $\hat{\rho}$
$\boldsymbol{\sigma}$	Shielding tensor
σ_j	(Isotropic) shielding constant of nucleus j
$\sigma_{\parallel}$, $\sigma_{\perp}$	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
$\tau_{\parallel}$, $\tau_{\perp}$	Correlation times for molecular tumbling parallel and perpendicular to the symmetry axis
χ	(i) Magnetic susceptibility; (ii) nuclear quadrupole coupling constant ($\chi = e^2 q_{ZZ} Q/h$)
$\omega_j, \omega_0, \omega_1, \omega_2$	As for ν_j, 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 $\boldsymbol{B}_1$, $\boldsymbol{B}_2$

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

NMR Tables

^{1}H Chemical Shifts for Common Contaminants in Deuterated Solvents

	Proton	mult., J	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
residual solvent H			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O		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	
t-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		
t-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_3CO	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_3CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH_2CH_3	q, 7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH_2CH_3	t, 7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
ethyl methyl ketone	CH_3CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH_2CH_3	q, 7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH_2CH_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	
n-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
n-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	

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

	Proton	mult.	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
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_2O	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(*o/p*)	m	7.17	7.1-7.2	7.18	7.02	7.1-7.3	7.16	
	CH(*m*)	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 $^{2}J_{H,D}$ = 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 CH_2 and the OH protons may be observed (J = 5 Hz). [e] In CD_3CN, 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 CH_3 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.

^{13}C Chemical Shifts for Common Contaminants in Deuterated Solvents

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
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	
t-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
t-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_3Ar	21.20	21.31	20.97	21.40	21.23	21.38	
	CH_3C	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

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

		$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
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_3CO	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_3CO	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_2CH_3	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH_2CH_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	
n-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
n-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-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_2O	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*)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(*o*)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH(*m*)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH(*p*)	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] $^2J_{PC}$ = 3 Hz. [c] Reference material; see text.

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NMR Formulae

Quantity	Formula (bold face = vectors)	Definitions (SI units) (see SI section for constants and units)
Magnetic Field Magnetic Force	$\boldsymbol{B} = \mu_o\ \boldsymbol{H}$ $\boldsymbol{F} = Q\ \boldsymbol{v}\times\boldsymbol{B}$	$\boldsymbol{B}$ = magn. flux density, magn. induction (T) $\boldsymbol{H}$ = magn. field strength (A m^{-1}) μ_o = permeability of vacuum ($4\pi\times10^{-7}$ H m^{-1}) Q = elec. charge (C); v = velocity (m/s)
Nuclear Spin Spin Angular Mom. Magn. Moment	$\boldsymbol{I}$ $\hbar\ m_I$ $\boldsymbol{\mu}_I = \gamma_I \hbar\ \boldsymbol{I} = g_I\beta_N\ \boldsymbol{I}$	γ = magnetogyric ratio (rad s^{-1} T^{-1}); $\hbar = h/2\pi$ $\beta_N = \mu_B$ (nuclear magneton); g_I = nuclear g factor m_I = quantum no. ($-I$, $-I$+1, ...+I)
Zeeman Interaction Larmor Freq. Nutation Vector	$\mathrm{H} = -\boldsymbol{\mu}_I \cdot \boldsymbol{B}_0$, $E = -m_I\ \gamma_I\ \hbar\ B_0$ $\omega_0 = \gamma_I B_0$, $\nu_0 = \nu_I\ B_0$ $\boldsymbol{\omega} = -\gamma_I\ \boldsymbol{B}$	ω in rad s^{-1}, ν in Hz ($\Delta m_I = \pm1$), $\nu = \gamma/2\pi$ (clockwise precession in lab frame for $\gamma > 0$)
Boltzmann Pop. Diff. Equil. Magn.	$\Delta N/N \sim \gamma_I\ \hbar/2kT\ (\Delta m_I = \pm1)$ $M_0 = B_0\ [N\gamma_I^2\hbar^2\ I(I+1)\ /\ 3kT]$	N = number of nuclei with spin I T = temperature (K)
Rotating Frame (r.f.) and residual field	$\gamma\ \Delta\boldsymbol{B}_0 = \gamma\ \boldsymbol{B}_0 + \boldsymbol{\omega}_{\mathbf{r.f.}}$ $\boldsymbol{\Omega} = -\gamma\ \Delta\boldsymbol{B}_0 = \boldsymbol{\omega}_{\mathbf{0}} - \boldsymbol{\omega}_{\mathbf{r.f.}}$	$\boldsymbol{\omega}_{\mathbf{r.f.}}$ = rot. frame vector (detector freq.) in direction $\boldsymbol{\omega}_{\mathbf{0}}$ ($-z$ axis for $\gamma > 0$) $\Delta\boldsymbol{B}_0$ = 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	$\boldsymbol{\omega}_1 = -\gamma\ \boldsymbol{B}_1$, $\boldsymbol{B}_{\mathbf{eff}} = \boldsymbol{B}_1 + \Delta\boldsymbol{B}_0$ $B_{eff} = [B_1^2 + \Delta B_0^2]^{1/2}$, $\tan\theta = \Delta B_0/B_1$ $\boldsymbol{\beta}_{\mathbf{eff}}$ (in rad) $= -\gamma\ \boldsymbol{B}_{\mathbf{eff}}\ \tau_p$ $\nu_{B_{eff}}$ (in Hz) $= 1/(4\tau_{90})$	$\boldsymbol{B}_1$ = RF field vector in xy plane; nutation is ccw around $\boldsymbol{\omega}_{\mathbf{eff}} = -\gamma\ \boldsymbol{B}_{\mathbf{eff}}$; θ = tilt angle between $\boldsymbol{B}_{\mathbf{eff}}$ and xy-plane; for $\Delta B_0/B_1 < 0.1$: $\theta < 6°$, $B_{eff} \approx B_1$ τ_p = RF pulse width (s); τ_{90} = 90° 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: $R_2 = 1/T_2 = \pi\Delta\nu_o$	$\Delta\nu_o$ = 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; $\omega_S\tau_C << 1$)	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 Formulae

NMR Relaxation

Mechanisms (isotropic tumbling, SI units)	**Remarks**
Intramolecular Heteronuclear Dipole-Dipole Spin I relaxed by Spin S $R_1^I = E_{IS}\, r_{IS}^{-6}\, [(1/12)J_0(\omega_I - \omega_S) + (3/2)J_1(\omega_I) + (3/4)J_2(\omega_I + \omega_S)]$ $R_2^I = E_{IS}\, r_{IS}^{-6}\, [(1/6)J_0(0) + (1/24)J_0(\omega_I - \omega_S) + (3/4)J_1(\omega_I) + (3/2)J_1(\omega_S) + (3/8)J_2(\omega_I + \omega_S)]$ where $E_{IS} = (\mu_0/4\pi)^2\, (\gamma_I\, \gamma_S\, \hbar)^2\, S(S+1)$ Extreme narrowing: $R_1^I = (4/3)\, E_{IS}\, r_{IS}^{-6}\, \tau_c\ (\omega\tau_c << 1)$ For several spins S: use $\sum r_{IS}^{-6}$ NB: $T_1^I = 1/R_1^I$ only when S is saturated	Factor $(\mu_0/4\pi) = 10^{-7}$ is required for conversion from cgs-Gauss units to MKSA (SI) units. Spectral Densities for random isotropic rotation $J_q(\omega) = C_q\, [\tau_c/(1 + \omega^2\tau_c^2)]$ $(q = 0,1,2)$ $C_0 = 24/15;\ C_1 = 4/15;\ C_2 = 16/15$ extreme narrowing: $J_q(\omega) = C_q\, \tau_c$
Intramolecular Homonuclear Dipole-Dipole Spin I_k relaxed by Spin I_1 $R_1^I = E_I\, r_{kl}^{-6}\, (3/2)\, [J_1(\omega_I) + J_2(2\omega_I)]$ $R_{1\rho}^I = E_I\, r_{kl}^{-6}\, [(3/8)J_0(\omega_1) + (15/4)J_1(\omega_I) + (3/8)J_2(2\omega_I)]$ $R_2^I = E_I\, r_{kl}^{-6}\, [(3/8)J_0(0) + (15/4)J_1(\omega_I) + (3/8)J_2(2\omega_I)]$ where $E_I = (\mu_0/4\pi)^2\, \gamma_I^4\, \hbar^2\, I(I+1)$ Extreme narrowing: $R_1^I = R_2^I = 2\, E_I\, r_{kl}^{-6}\, \tau_c\ (\omega\tau_c << 1)$ For several spins I: use $\sum r_{kl}^{-6}$	
Intermolecular Heteronuclear Dipole-Dipole Spin I on mol. A relaxed by Spin S on mol. B $(\omega\tau_C << 1)$ $R_1^I = 16\pi\, c_S\, E_{IS} / (27\, r_{IS}\, D_{trans})$ (pair distribution function = step function)	$E_{IS} = (\mu_0/4\pi)^2\, (\gamma_I\, \gamma_S\, \hbar)^2\, S(S+1)$ c_S = conc. of spins S r_{IS} = distance of closest approach $D_{trans} = (D_A + D_B)/2$
Intermolecular Homonuclear Dipole-Dipole Spin I on mol. A relaxed by Spin I on mol. B $(\omega\tau_C << 1)$ $R_1^I = 8\pi c_I\, E_I / (9\, r_{II}\, D_{trans})$ also found in the literature is: $R_1^I = (4\pi/3)\, c_I\, E_I\, (\tau/r_{II}^3)\, [1 + (2r_{II}^2/5\, D_{trans}\, \tau)]$	$E_I = (\mu_0/4\pi)^2\, \gamma_I^4\, \hbar^2\, I(I+1)$ c_I = conc. of spins I r_{II} = distance of closest approach τ = mol. jump time

Spherical Harmonics

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

$Y_{0,0}$	$=$	$\sqrt{\frac{1}{4\pi}}$		
$Y_{1,0}$	$=$	$\sqrt{\frac{3}{4\pi}}\cos\theta$	$=$	$\sqrt{\frac{3}{4\pi}}\,\frac{z}{r}$
$Y_{1,\pm1}$	$=$	$\mp\sqrt{\frac{3}{8\pi}}\sin\theta\ e^{\pm i\varphi}$	$=$	$\mp\sqrt{\frac{3}{8\pi}}\,\frac{x\pm iy}{r}$
$Y_{2,0}$	$=$	$\sqrt{\frac{5}{16\pi}}\ (3\cos^2\theta - 1)$	$=$	$\sqrt{\frac{5}{16\pi}}\,\frac{2z^2 - x^2 - y^2}{r^2}$
$Y_{2,\pm1}$	$=$	$\mp\sqrt{\frac{15}{8\pi}}\cos\theta\ \sin\theta\ e^{\pm i\varphi}$	$=$	$\mp\sqrt{\frac{15}{8\pi}}\,\frac{(x\pm iy)z}{r^2}$
$Y_{2,\pm2}$	$=$	$\sqrt{\frac{15}{32\pi}}\ \sin^2\theta\ e^{\pm 2i\varphi}$	$=$	$\sqrt{\frac{15}{32\pi}}\,\frac{(x\pm iy)^2}{r^2}$

NMR Formulae

Mechanisms (isotropic tumbling, SI units)	**Remarks**
Chemical Shift Anisotropy (CSA) molecular tumbling modulates the interaction of the chem. shift tensor with the B_0 field. $R_1 = (2/5)\ E_{CSA}\ [\tau_c / (1 + \omega^2\tau_c^2)]$ $R_2 = (1/90)\ E_{CSA}\ \{8\tau_c + [6\tau_c + (1 + \omega^2\tau_c^2)]\}$	predominant relaxation mech. for non-protonated X nuclei $E_{CSA} = \gamma^2\ B_0^2\ \Delta\sigma^2$ $\Delta\sigma = \sigma_\perp - \sigma_\parallel$ (in ppm) (assuming axial symmetry of tensor)
Quadrupole Relaxation ($I > 1/2$) $R_1 = R_2 = (3/40)\ C_i\ [1 + \eta^2/3]\ C_{QF}^2\ \tau_c \quad (\omega\tau_c << 1)$	$C_i = (2I + 3) / [I^2(2I - 1)]$ $C_{QF} = e^2\ Q\ q_{zz} / \hbar$ = quadrupolar coupling in Hz; η = asymmetry param.
Spin-Rotation Interaction (SR) 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: $\left(\frac{1}{T_1}\right)_{SR} = \frac{2\ I_i\ kT}{3\ \hbar^2}\ C_{eff}^2\ \tau_J$ I_i = moment of inertia of the molecule C_{eff} = effective spin-rotational coupling constant τ_J = angular momentum correlation time With $\tau_c \cdot \tau_J = \frac{I_i}{6kT}$, we can introduce the reorientational correlation time and we obtain: $\left(\frac{1}{T_1}\right)_{SR} = \frac{I_i^2}{9\ \hbar^2}\ C_{eff}^2 \cdot \frac{1}{\tau_c}$	
Scalar Coupling (SC) This relaxation mechanism can occur if the nucleus I in question is scalar coupled (with coupling constant J) to a second spin ($S \geqq ½$) and the coupling is modulated by either chemical exchange (**SC relaxation of the first kind**) or the relaxation of spin S, e.g. if $S > ½$, (**SC relaxation of the second kind**). In this case spin splittings disappear and single lines are observed. $\left(\frac{1}{T_1}\right)_{SC} = \frac{8\pi^2\ J^2\ S\ (S+1)}{3}\ \left[\frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2\ \tau_{SC}^2}\right]$ $\left(\frac{1}{T_2}\right)_{SC} = \frac{4\pi^2\ J^2\ S\ (S+1)}{3}\ \left[\tau_{SC} + \frac{\tau_{SC}}{1 + (\omega_I - \omega_S)^2\ \tau_{SC}^2}\right]$ τ_{SC} = τ_e, if exchange time $\tau_e \ll T_1$ of either spin (first kind) τ_{SC} = T_1^S (the relaxation time of spin S) if $T_1^S \ll \tau_e$, $1/2\pi J$ (second kind) 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.	

X-ray Diffractometry Tables

Bond Lengths of Main Group Elements

	H	B	C	N	O	F		Al	Si	P	S	Cl		Ga	Ge	As	Se	Br		In	Sn	Sb	Te	I
H	**68**	115	111	99	92	86		152	147	143	135	130		152	154	154	148	144		176	172	174	169	167
B	115	**162**	157	145	138	131		199	195	190	181	176		199	201	200	194	191		224	219	221	216	213
C	111	157	**158**	148	143	137		192	188	185	182	178		193	196	197	195	193		216	213	215	211	210
N	99	145	148	**146**	142	138		179	175	173	172	173		180	184	186	185	186		203	200	202	199	199
O	92	138	143	142	**144**	142		171	168	167	166	168		173	177	180	179	181		195	193	195	192	193
F	86	131	137	138	142	**148**		163	161	160	160	163		166	170	173	173	176		187	185	188	185	186
Al	152	199	192	179	171	163		**244**	236	227	217	210		239	238	237	229	225		268	261	261	253	249
Si	147	195	188	175	168	161		236	**230**	222	213	206		234	234	232	225	222		260	255	256	249	245
P	143	190	185	173	167	160		227	222	**218**	210	204		227	229	228	222	219		251	247	249	244	241
Si	135	181	182	172	166	160		217	213	210	**206**	202		218	220	222	219	216		241	238	240	235	235
Cl	130	176	178	173	168	163		210	206	204	202	**202**		211	215	217	215	216		234	231	233	230	230
Ga	152	199	193	180	173	166		239	234	227	218	211		**238**	238	237	230	226		263	259	260	253	250
Ge	154	201	196	184	177	170		238	234	229	220	215		238	**240**	239	233	230		263	258	260	255	252
As	154	200	197	186	180	173		237	232	228	222	217		237	239	**240**	235	231		261	257	259	254	253
Se	148	194	195	185	179	173		229	225	222	219	215		230	233	235	**232**	230		254	250	252	248	248
Br	144	191	193	186	181	176		225	222	219	216	216		226	230	231	230	**230**		249	246	248	245	245
In	175	223	216	202	195	187		268	260	251	241	234		263	262	260	253	249		**292**	285	285	277	273
Sn	172	219	213	200	193	185		261	255	247	238	231		259	258	257	250	246		285	**280**	281	273	270
Sb	174	221	215	202	195	188		261	256	249	240	233		260	260	259	252	248		285	281	**282**	275	272
Te	169	216	211	199	192	185		253	249	244	235	230		253	255	254	248	245		278	273	275	**270**	267
I	167	213	210	199	193	186		249	245	241	235	230		250	252	253	248	245		274	270	272	267	**266**

Bond valences s may be calculated from experimental bond lengths (d) after Pauling's correlation equation (Pauling, The Nature of Chemical Bond) using this single bond length (d_0). The constant b is commonly taken to be 37 pm.

$$s = \exp\left[(d_0 - d)/b\right] \qquad d = d_0 - (b \ln s)$$

The single bond lengths are listed in pm. They are calculated from the modified Schomaker-Stevenson equation (Blom, Haaland, *J. Mol. Struc.* 128 (1985) 21-27).

Laue Classes and Point Groups

Crystal System	Laue Class	Point Group
Triclinic	-1	*1* -1
Monoclinic	2/m	*2* m 2/m
Orthorhombic	mmm	*222* mm2 mmm
Tetragonal	4/m 4/mmm	*4* -4 4/m *422* -42m 4mm 4/mmm
Trigonal/Hexagonal	-3 -3m1 (-31m) 6/m 6/mmm	*3* -3 *321 (312)* 3m1 (31m) -3m1 (-31m) *6* -6 6/m *622* -62m 6mm 6/mmm
Cubic	m-3 m-3m	*23* m-3 *432* -43m m-3m

X-ray Diffractometry Tables

Space Groups

Point groups and space groups without centers of inversion or mirror planes are printed in italics. Those space groups which are uniquely determinable from the systematic absences and the symmetry of the diffraction pattern are printed in bold type.

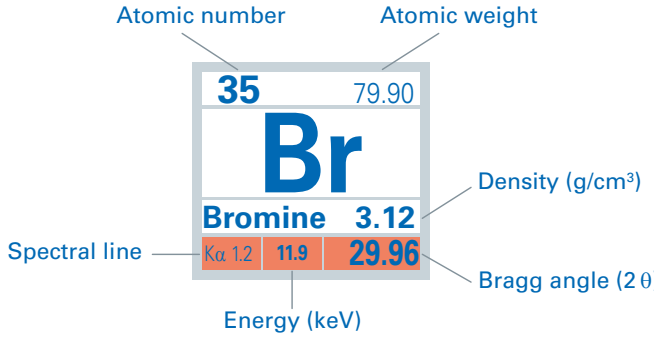
Crystal System	Point Group	SG #	Condensed Symbol	Full Symbol
triclinic	*1*	*1*	*P1*	
	-1	2	P-1	
monoclinic	*2*	*3*	*P2*	*P 1 2 1*
		4	*P2(1)*	*P 1 2(1) 1*
		5	*C2*	*C 1 2 1*
	m	6	Pm	P 1 m 1
		7	Pc	P 1 c 1
		8	Cm	C 1 m 1
		9	Cc	C 1 c 1
	2/m	10	P2/m	P 1 2/m 1
		11	P2(1)/m	P 1 2(1)/m 1
		12	C2/m	C 1 2/m 1
		13	P2/c	P 1 2/c 1
		14	**P2(1)/c**	**P 1 2(1)/c 1**
		15	C2/c	C 1 2/c 1
orthorhombic	*222*	*16*	*P222*	*P 2 2 2*
		17	***P222(1)***	***P 2 2 2(1)***
		18	***P2(1)2(1)2***	***P 2(1)2(1) 2***
		19	***P2(1)2(1)2(1)***	***P 2(1) 2(1) 2(1)***
		20	***C222(1)***	***C 2 2 2(1)***
		21	*C222*	*C 2 2 2*
		22	*F222*	*F 2 2 2*
		23	*I222*	*I 2 2 2*
		24	*I2(1)2(1)2(1)*	*I 2(1) 2(1) 2(1)*
	mm2	25	Pmm2	P m m 2
		26	Pmc2(1)	P m c 2(1)
		27	Pcc2	P c c 2
		28	Pma2	P m a 2
		29	Pca2(1)	P c a 2(1)
		30	Pnc2	P n c 2
		31	Pmn2(1)	P m n 2(1)
		32	Pba2	P b a 2
		33	Pna2(1)	P n a 2(1)
		34	Pnn2	P n n 2
		35	Cmm2	C m m 2
		36	Cmc2(1)	C m c 2(1)
		37	Ccc2	C c c 2
		38	Amm2	A m m 2
		39	Abm2	A b m 2
		40	Ama2	A m a 2
		41	Aba2	A b a 2
		42	Fmm2	F m m 2
		43	**Fdd2**	**F d d 2**
		44	Imm2	I m m 2
		45	Iba2	I b a 2
		46	Ima2	I m a 2
	mmm	47	Pmmm	P 2/m 2/m 2/m
		48	**Pnnn**	**P 2/n 2/n 2/n**
		49	Pccm	P 2/c 2/c 2/m
		50	**Pban**	**P 2/b 2/a 2/n**
		51	Pmma	P 2(1)/m 2/m 2/a
		52	**Pnna**	**P 2/n 2(1)/n 2/a**
		53	Pmna	P 2/m 2/n 2(1)/a
		54	**Pcca**	**P 2(1)/c 2/c 2/a**
		55	Pbam	P 2(1)/b 2(1)/a 2/m
		56	**Pccn**	**P 2(1)/c 2(1)/c 2/n**
		57	Pbcm	P 2/b 2(1)/c 2(1)/m
		58	Pnnm	P 2(1)/n 2(1)/n 2/m
		59	Pmmn	P 2(1)/m 2(1)/m 2/n
		60	**Pbcn**	**P 2(1)/b 2/c 2(1)/n**
		61	**Pbca**	**P 2(1)/b 2(1)/c 2(1)/a**
		62	Pnma	P 2(1)/n 2(1)/m 2(1)/a
		63	Cmcm	C 2/m 2/c 2(1)/m
		64	Cmca	C 2/m 2/c 2(1)/a
		65	Cmmm	C 2/m 2/m 2/m
		66	Cccm	C 2/c 2/c 2/m
		67	Cmma	C 2/m 2/m 2/a
		68	**Ccca**	**C 2/c 2/c 2/a**
		69	Fmmm	F 2/m 2/m 2/m
		70	**Fddd**	**F 2/d 2/d 2/d**
		71	Immm	I 2/m 2/m 2/m
		72	Ibam	I 2/b 2/a 2/m
		73	Ibca	I 2(1)/b 2(1)/c 2(1)/a
		74	Imma	I 2(1)/m 2(1)/m 2(1)/a
tetragonal	*4*	*75*	*P4*	*P 4*
		76	***P4(1)***	***P 4(1)***
		77	*P4(2)*	*P 4(2)*
		78	***P4(3)***	***P 4(3)***
		79	*I4*	*I 4*
		80	***I4(1)***	***I 4(1)***
	-4	81	P-4	P -4
		82	I-4	I -4
	4/m	83	P4/m	P 4/m
		84	P4(2)/m	P 4 (2)/m
		85	**P4/n**	**P 4/n**
		86	**P4(2)/n**	**P 4(2)/n**
		87	I4/m	I 4/m
		88	**I4(1)/a**	**I 4(1)/a**
	422	*89*	*P422*	*P 4 2 2*
		90	***P42(1)2***	***P 4 2(1) 2***
		91	*P4(1)22*	*P 4(1) 2 2*
		92	***P4(1)2(1)2***	***P 4(1) 2(1) 2***
		93	***P4(2)22***	***P 4(2)2 2***
		94	***P4(2)2(1)2***	***P 4(2) 2(1) 2***
		95	***P4(3)22***	***P 4(3) 2 2***
		96	***P4(3)2(1)2***	***P 4(3) 2(1) 2***
		97	*I422*	*I 4 2 2*
		98	***I4(1)22***	***I 4(1) 2 2***
	4mm	99	P4mm	P 4 m m
		100	P4bm	P 4 b m
		101	P4(2)cm	P 4(2) c m
		102	P4(2)nm	P 4(2) n m
		103	P4cc	P 4 c c
		104	P4nc	P 4 n c
		105	P4(2)mc	P 4(2) m c
		106	P4(2)bc	P 4(2) b c
		107	I4mm	I 4 m m
		108	I4cm	I 4 c m
		109	I4(1)md	I 4(1) m d
		110	**I4(1)cd**	**I 4(1) c d**
	-42m	111	P-42m	P -4 2 m
		112	P-42c	P -4 2 c
		113	P-42(1)m	P -4 2(1) m
		114	**P-42(1)c**	**P -4 2(1) c**
		115	P-4m2	P -4 m 2
		116	P-4c2	P -4 c 2
		117	P-4b2	P -4 b 2
		118	P-4n2	P -4 n 2
		119	I-4m2	I -4 m 2
		120	I-4c2	I -4 c 2
		121	I-42m	I -4 2 m
		122	I-42d	I -4 2 d
	4/mmm	123	P4/mmm	P 4/m 2/m 2/m
		124	P4/mcc	P 4/m 2/c 2/c
		125	**P4/nbm**	**P 4/n 2/b 2/m**

X-ray Diffractometry Tables

Crystal System	Point Group	SG #	Condensed Symbol	Full Symbol
		126	**P4/nnc**	**P 4/n 2/n 2/c**
		127	P4/mbm	P 4/m 2(1)/b 2/m
		128	P4/mnc	P 4/m 2(1)/n 2/c
		129	**P4/nmm**	**P 4/n 2(1)/m 2/m**
		130	**P4/ncc**	**P 4/n 2(1)/c 2/c**
		131	P4(2)/mmc	P 4(2)/m 2/m 2/c
		132	P4(2)/mcm	P 4(2)/m 2/c 2/m
		133	**P4(2)/nbc**	**P 4(2)/n 2/b 2/c**
		134	**P4(2)/nnm**	**P 4(2)/n 2/n 2/m**
		135	P4(2)/mbc	P 4(2)/m 2(1)/b 2/c
		136	P4(2)/mnm	P 4(2)/m 2(1)/n 2/m
		137	**P4(2)/nmc**	**P 4(2)/n 2(1)/m 2/c**
		138	**P4(2)/ncm**	**P 4(2)/n 2(1)/c 2/m**
		139	I4/mmm	I 4/m 2/m 2/m
		140	I4/mcm	I 4/m 2/c 2/m
		141	**I4(1)/amd**	**I 4(1)/a 2/m 2/d**
		142	**I4(1)/acd**	**I 4(1)/a 2/c 2/d**
trigonal	*3*	*143*	*P3*	*P 3*
		144	*P3(1)*	*P 3(1)*
		145	*P3(2)*	*P 3(2)*
		146	*R3*	*R 3*
	-3	147	P-3	P -3
		148	R-3	R -3
	32	*149*	*P312*	*P 3 1 2*
		150	*P321*	*P 3 2 1*
		151	***P3(1)12***	***P 3(1) 1 2***
		152	***P3(1)21***	***P 3(1) 2 1***
		153	***P3(2)12***	***P 3(2) 1 2***
		154	***P3(2)21***	***P 3(2) 2 1***
		155	*R32*	*R 3 2*
	3m	156	P3m1	P 3 m 1
		157	P31m	P 3 1 m
		158	P3c1	P 3 c 1
		159	P31c	P 3 1 c
		160	R3m	R 3 m
		161	R3c	R 3 c
	-3m	162	P-31m	P -3 1 2/m
		163	P-31c	P -3 1 2/c
		164	P-3m1	P -3 2/m 1
		165	P-3c1	P -3 2/c 1
		166	R-3m	R -3 2/m
		167	R-3c	R -3 2/c
hexagonal	*6*	*168*	*P6*	*P 6*
		169	***P6(1)***	***P 6(1)***
		170	***P6(5)***	***P 6(5)***
		171	***P6(2)***	***P 6(2)***
		172	***P6(4)***	***P 6(4)***
		173	*P6(3)*	*P 6(3)*
	-6	174	P-6	P -6
	6/m	175	P6/m	P 6/m
		176	P6(3)/m	P 6(3)/m
	622	*177*	*P622*	*P 6 2 2*
		178	***P6(1)22***	***P 6(1)2 2***
		179	***P6(5)22***	***P 6(5) 2 2***
		180	***P6(2)22***	***P 6(2) 2 2***
		181	***P6(4)22***	***P 6(4) 2 2***
		182	***P6(3)22***	***P 6(3) 2 2***
	6mm	183	P6mm	P 6 m m
		184	P6cc	P 6 c c
		185	P6(3)cm	P 6(3) c m
		186	P6(3)mc	P 6(3) m c
	-6m	187	P-6m2	P -6 m 2
		188	P-6c2	P -6 c 2
		189	P-62m	P -6 2 m
		190	P-62c	P -6 2 c
	6/mmm	191	P6/mmm	P 6/m 2/m 2/m
		192	P6/mcc	P 6/m 2/c 2/c
		193	P6(3)/mcm	P 6(3)/m 2/c 2/m
		194	P6(3)/mmc	P 6(3)/m 2/m 2/c

Crystal System	Point Group	SG #	Condensed Symbol	Full Symbol
cubic	*23*	*195*	*P23*	*P 2 3*
		196	*F23*	*F 2 3*
		197	*I23*	*I 2 3*
		198	***P2(1)3***	***P 2(1) 3***
		199	*I2(1)3*	*I 2(1) 3*
	m-3	200	Pm-3	P 2/m -3
		201	**Pn-3**	**P 2/n -3**
		202	Fm-3	F 2/m -3
		203	**Fd-3**	**F 2/d -3**
		204	Im-3	I 2/m -3
		205	**Pa-3**	**P 2(1)/a -3**
		206	**Ia-3**	**I 2(1)/a -3**
	432	*207*	*P432*	*P 4 3 2*
		208	***P4(2)32***	***P 4(2) 3 2***
		209	*F432*	*F 4 3 2*
		210	***F4(1)32***	***F 4(1) 3 2***
		211	*I432*	*I 4 3 2*
		212	***P4(3)32***	***P 4(3) 3 2***
		213	***P4(1)32***	***P 4(1) 3 2***
		214	*I4(1)32*	*I 4(1) 3 2*
	-43m	215	P-43m	P -4 3 m
		216	F-43m	F -4 3 m
		217	I-43m	I -4 3 m
		218	P-43n	P -4 3 n
		219	F-43c	F -4 3 c
		220	**I-43d**	**I -4 3 d**
	m-3m	221	Pm-3m	P 4/m -3 2/m
		222	**Pn-3n**	**P 4/n -3 2/n**
		223	Pm-3n	P 4(2)/m -3 2/n
		224	**Pn-3m**	**P 4(2)/n -3 2/m**
		225	Fm-3m	F 4/m -3 2/m
		226	Fm-3c	F 4/m -3 2/c
		227	**Fd-3m**	**F 4(1)/d -3 2/m**
		228	**Fd-3c**	**F 4(1)/d -3 2/c**
		229	Im-3m	I 4/m -3 2/m
		230	**Ia-3d**	**I 4(1)/a -3 2/d**

Periodic Table of Elements for X-ray Applications



1	1.01		
H			
Hydrogen	0.0007		

3	6.94		
Li			
Lithium	0.534		

4	9.01		
Be			
Beryllium	1.85		
Kα 1.2	0.109	74.34	

11	22.99		
Na			
Sodium	0.97		
Kα 1.2	1.0	25.00	
Kα 1.2	1.0	55.08	
Kβ 1	1.1	24.40	

12	24.31		
Mg			
Magnesium	1.74		
Kα 1.2	1.3	20.70	
Kα 1.2	1.3	136.72	
Kβ 1	1.3	20.00	

19	39.10		
K			
Potassium	0.86		
Kα 1.2	3.3	136.67	
Kα 1.2	3.3	50.69	
Kβ 1	3.6	118.10	

20	40.08		
Ca			
Calcium	1.54		
Kα 1.2	3.7	113.07	
Kα 1.2	3.7	45.20	
Kβ 1	4.0	100.21	
Lα 1	0.3	82.68	
Lβ 1	0.3	81.61	

21	44.96		
Sc			
Scandium	2.99		
Kα 1.2	4.1	97.68	
Kα 1.2	4.1	40.59	
Kβ 1	4.5	87.28	
Lα 1	0.4	69.50	
Lβ 1	0.4	68.67	

22	47.87		
Ti			
Titanium	4.54		
Kα 1.2	4.5	86.12	
Kα 1.2	4.5	36.67	
Kβ 1	4.9	77.25	
Lα 1	0.5	59.83	
Lβ 1	0.5	58.97	

23	50.94		
V			
Vanadium	6.11		
Kα 1.2	5.0	76.92	
Kα 1.2	5.0	123.17	
Kβ 1	5.4	69.12	
Lα 1	0.5	52.35	
Lβ 1	0.5	51.49	

24	52.00		
Cr			
Chromium	7.15		
Kα 1.2	5.4	69.34	
Kα 1.2	5.4	107.11	
Kβ 1	6.0	62.35	
Lα 1	0.6	46.33	
Lβ 1	0.6	45.49	

25	54.94		
Mn			
Manganese	7.44		
Kα 1.2	5.9	62.96	
Kα 1.2	5.9	95.20	
Kβ 1	6.5	56.63	
Lα 1	0.6	41.45	
Lβ 1	0.6	40.65	

26	55.85		
Fe			
Iron	7.87		
Kα 1.2	6.4	57.51	
Kα 1.2	6.4	85.73	
Kβ 1	7.1	51.72	
Lα 1	0.7	37.30	
Lβ 1	0.7	36.60	

27	58.93		
Co			
Cobalt	8.56		
Kα 1.2	6.9	52.79	
Kα 1.2	6.9	77.89	
Kβ 1	7.7	47.46	
Lα 1	0.8	33.77	
Lβ 1	0.8	33.12	

37	85.47		
Rb			
Rubidium	1.53		
Kα 1.2	13.4	26.61	
Kα 1.2	13.4	37.99	
Kβ 1	15.0	23.75	
Lα 1	1.7	113.68	
Lβ 1	1.8	108.08	
Kα 1.2	13.4	62.00	
Kβ 1	15.0	54.79	

38	87.62		
Sr			
Strontium	2.64		
Kα 1.2	14.1	25.15	
Kα 1.2	14.1	35.85	
Kβ 1	15.8	22.42	
Lα 1	1.8	103.45	
Lβ 1	1.9	98.53	
Kα 1.2	14.1	58.31	
Kβ 1	15.8	51.54	

39	88.91		
Y			
Yttrium	4.47		
Kα 1.2	14.9	23.79	
Kα 1.2	14.9	33.90	
Kβ 1	16.7	21.19	
Lα 1	1.9	95.07	
Lβ 1	2.0	90.57	
Kα 1.2	14.9	54.95	
Kβ 1	16.7	48.57	

40	91.22		
Zr			
Zirconium	6.51		
Kα 1.2	15.8	22.50	
Kα 1.2	15.8	32.04	
Kβ 1	17.7	20.07	
Lα 1	2.0	87.96	
Lβ 1	2.1	83.76	
Kα 1.2	15.8	51.75	
Kβ 1	17.7	45.28	

41	92.91		
Nb			
Niobium	8.57		
Kα 1.2	16.6	21.35	
Kα 1.2	16.6	30.38	
Kβ 1	18.6	19.03	
Lα 1	2.2	81.81	
Lβ 1	2.3	77.84	
Kα 1.2	16.6	48.35	
Kβ 1	18.6	43.39	

42	95.94		
Mo			
Molybdenum	10.22		
Kα 1.2	17.5	20.28	
Kα 1.2	17.5	28.84	
Kβ 1	19.6	18.06	
Lα 1	2.3	76.41	
Lβ 1	2.4	72.63	
Kα 1.2	17.5	46.39	
Kβ 1	19.6	41.11	

43	(98)		
Tc			
Technetium	11.5		
Kα 1.2	18.4	19.29	
Kα 1.2	18.4	27.42	
Kβ 1	20.6	17.17	
Lα 1	2.4	71.62	
Lβ 1	2.5	67.98	
Kα 1.2	18.4	44.03	
Kβ 1	20.6	39.01	

44	101.07		
Ru			
Ruthenium	12.37		
Kα 1.2	19.3	18.37	
Kα 1.2	19.3	26.10	
Kβ 1	21.7	16.34	
Lα 1	2.6	67.33	
Lβ 1	2.7	63.82	
Kα 1.2	19.3	41.84	
Kβ 1	21.7	37.07	

45	102.91		
Rh			
Rhodium	12.41		
Kα 1.2	20.2	17.51	
Kα 1.2	20.2	24.87	
Kβ 1	22.7	15.57	
Lα 1	2.7	63.46	
Lβ 1	2.8	60.05	
Kα 1.2	20.2	39.82	
Kβ 1	22.7	35.51	

55	132.91		
Cs			
Caesium	1.87		
Kα 1	30.9	16.16	
Lα 1	4.3	91.80	
Lβ 1	4.6	83.58	

56	137.33		
Ba			
Barium	3.59		
Kα 1	32.1	15.54	
Lα 1	4.5	87.16	
Lβ 1	4.8	79.24	

57	138.91		
La			
Lanthanium	6.15		
Kα 1	33.4	14.96	
Lα 1	4.7	82.90	
Lβ 1	5.0	75.27	

72	178.49		
Hf			
Hafnium	13.31		
Kα 1	55.8	8.95	
Lα 1	7.9	45.87	
Lβ 1	9.0	39.90	
Mα 1	1.6	119.17	
Lα 1	7.9	121.27	
Lβ 1	9.0	99.46	

73	180.95		
Ta			
Tantalum	16.65		
Kα 1	57.6	8.68	
Lα 1	8.2	44.41	
Lβ 1	9.3	38.47	
Mα 1	1.7	112.11	
Lα 1	8.1	115.36	
Lβ 1	9.3	94.92	

74	183.84		
W			
Tungsten	19.25		
Lα 1	8.4	43.01	
Lβ 1	9.7	37.12	
Mα 1	1.8	106.03	
Lα 1	8.4	110.13	
Lβ 1	9.7	90.75	

75	186.21		
Re			
Rhenium	21.02		
Lα 1	8.7	41.68	
Lβ 1	10.0	35.82	
Mα 1	1.8	100.66	
Lα 1	8.7	105.43	
Lβ 1	10.0	86.90	

76	190.23		
Os			
Osmium	22.61		
Lα 1	8.9	40.42	
Lβ 1	10.4	34.59	
Mα 1	1.9	95.64	
Lα 1	8.9	101.16	
Lβ 1	10.4	83.33	

77	192.22		
Ir			
Iridium	22.65		
Lα 1	9.2	39.21	
Lβ 1	10.7	33.42	
Mα 1	2.0	91.50	
Lα 1	9.2	97.24	
Lβ 1	10.7	80.01	

87	(223)		
Fr			
Francium	1.87		
Lα 1	12.0	29.65	
Lβ 1	14.8	24.06	

88	(226)		
Ra			
Radium	5.5		
Lα 1	12.3	28.89	
Lβ 1	15.2	23.31	

89	(227)		
Ac			
Actinium	10.07		
Lα 1	12.7	28.17	
Lβ 1	15.7	22.59	

Lanthanides, Actinides:

58	140.12		
Ce			
Cerium	6.77		
Lα 1	4.8	128.13	
Lα 1	4.8	79.00	
Lβ 1	5.3	71.61	

59	140.91		
Pr			
Praseodymium	6.77		
Lα 1	5.0	119.69	
Lα 1	5.0	75.41	
Lβ 1	5.5	68.23	

60	144.24		
Nd			
Neodymium	7.01		
Lα 1	5.2	112.66	
Lα 1	5.2	72.12	
Lβ 1	5.7	65.10	

61	(145)		
Pm			
Promethium	7.26		
Lα 1	5.4	106.48	
Lα 1	5.4	69.03	
Lβ 1	6.0	62.19	

62	150.36		
Sm			
Samarium	7.52		
Lα 1	5.6	101.12	
Lα 1	5.6	66.22	
Lβ 1	6.2	59.49	

90	232.04		
Th			
Thorium	11.72		
Lα 1	13.0	39.22	
Lα 1	13.0	27.46	
Lβ 1	16.2	21.90	
Lα 1	13.0	64.12	
Lβ 1	16.2	50.29	

91	231.04		
Pa			
Protactinium	15.37		
Lα 1	13.3	38.23	
Lα 1	13.3	26.79	
Lβ 1	16.7	21.24	
Lα 1	13.3	62.39	
Lβ 1	16.7	48.68	

92	238.03		
U			
Uranium	18.45		
Lα 1	13.6	37.29	
Lα 1	13.6	26.14	
Lβ 1	17.2	20.59	
Lα 1	13.6	60.75	
Lβ 1	17.2	47.13	

93	(237)		
Np			
Neptunium	20.25		
Lα 1	14.0	36.38	
Lα 1	14.0	25.51	
Lβ 1	17.8	19.96	

94	(244)		
Pu			
Plutonium	19.84		
Lα 1	14.3	35.50	
α	14.3	24.90	
Lβ 1	18.3	19.39	

Analyser crystal	Name, material	2d-value (nm)
XS-B	La/B_4C multilayer	19.0
XS-C	$Ti0_2/C$ multilayer	12.0
XS-N	Ni/BN multilayer	11.0
XS-55	W/Si multilayer	5.5
XS-CEM	Specific structure	2.75
TIAP	Thallium biphthalate	2.576
ADP	Ammonium dihydrogen phosphate	1.064
PET	Pentaerythrite	0.874
InSb	Indium antimonide	0.748
Ge	Germanium	0.653
LiF (200)	Lithium fluoride	0.403
LiF (220)	Lithium fluoride	0.285
LiF (420)	Lithium fluoride	0.180

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$$\lambda\ (\text{nm}) = \frac{1.24}{E\ (\text{keV})}$$

$$n\lambda = 2d \sin\theta$$

2	4.00		
He			
Helium	0.0002		

5	10.81		
B			
Boron	2.34		
Kα 1,2	0.18	42.51	

6	12.01		
C			
Carbon	2.27		
Kα 1,2	0.28	107.24	
Kα 1,2	0.28	43.31	

7	14.01		
N			
Nitrogen	0.001		
Kα 1,2	0.39	70.14	
Kα 1,2	0.39	33.60	

8	16.00		
O			
Oxygen	0.001		
Kα 1,2	0.53	50.90	
Kα 1,2	0.53	25.10	

9	19.00		
F			
Fluorine	0.001		
Kα 1,2	0.68	38.91	
Kα 1,2	0.68	90.60	

10	20.18		
Ne			
Neon	0.0009		
Kα 1,2	0.85	30.8	
Kα 1,2	0.85	69.1	

13	26.98		
Al			
Aluminium	2.70		
Kα 1,2	1.5	145.12	
Kα 1,2	1.5	17.45	
Kβ 1	1.5	131.86	
Kα 1	1.5	35.31	

14	28.09		
Si			
Silicon	2.33		
Kα 1,2	1.7	109.21	
Kα 1,2	1.7	144.58	
Kβ 1	1.8	101.67	
Kα 1	1.7	30.04	

15	30.97		
P			
Phosphorus	1.82		
Kα 1,2	2.0	89.56	
Kα 1,2	2.0	141.03	
Kβ 1	2.1	83.20	
Kα 1	2.0	25.88	

16	32.07		
S			
Sulphur	2.07		
Kα 1,2	2.3	75.85	
Kα 1,2	2.3	110.69	
Kβ 1	2.5	70.28	
Kα 1	2.3	22.53	

17	35.45		
Cl			
Chlorine	0.003		
Kα 1,2	2.6	65.49	
Kα 1,2	2.6	92.76	
Kβ 1	2.8	60.49	

18	39.95		
Ar			
Argon	0.002		
Kα 1,2	3.0	57.32	
Kα 1,2	3.0	79.86	
Kβ 1	3.2	52.79	

28	58.69		
Ni			
Nickel	8.91		
Kα 1,2	7.5	48.67	
Kα 1,2	7.5	71.26	
Kβ 1	8.3	43.72	
Lα 1	0.9	30.70	
Lβ 1	0.9	30.08	
Kα 1,2	7.5	134.33	
Kβ 1	8.3	112.81	

29	63.55		
Cu			
Copper	8.93		
Kα 1,2	8.0	45.02	
Kα 1,2	8.0	65.55	
Kβ 1	8.9	40.45	
Lα 1	0.9	28.06	
Lβ 1	1.0	27.45	
Kα 1,2	8.0	117.85	
Kβ 1	8.9	101.26	

30	65.41		
Zn			
Zinc	7.13		
Kα 1,2	8.6	41.80	
Kα 1,2	8.6	60.58	
Kβ 1	9.6	37.52	
Lα 1	1.0	25.74	
Lβ 1	1.0	25.18	
Kα 1,2	8.6	105.87	
Kβ 1	9.6	91.98	

31	69.72		
Ga			
Gallium	5.91		
Kα 1,2	9.2	38.91	
Kα 1,2	9.2	56.20	
Kβ 1	10.3	34.90	
Lα 1	1.1	23.69	
Lβ 1	1.1	23.12	
Kα 1,2	9.2	96.35	
Kβ 1	10.3	84.24	

32	72.64		
Ge			
Germanium	5.32		
Kα 1,2	9.9	36.32	
Kα 1,2	9.9	52.31	
Kβ 1	11.0	32.56	
Lα 1	1.2	21.88	
Lβ 1	1.2	21.33	
Kα 1,2	9.9	88.44	
Kβ 1	11.0	77.64	

33	74.92		
As			
Arsenic	5.78		
Kα 1,2	10.5	33.99	
Kα 1,2	10.5	48.83	
Kβ 1	11.7	30.44	
Lα 1	1.3	20.25	
Lβ 1	1.3	19.71	
Kα 1,2	10.5	81.69	
Kβ 1	11.7	71.90	

34	78.96		
Se			
Selenium	4.81		
Kα 1,2	11.2	31.89	
Kα 1,2	11.2	45.71	
Kβ 1	12.5	28.52	
Lα 1	1.4	18.82	
Lβ 1	1.4	18.28	
Kα 1,2	11.2	75.84	
Kβ 1	12.5	66.86	

35	79.90		
Br			
Bromine	3.12		
Kα 1,2	11.9	29.96	
Kα 1,2	11.9	42.88	
Kβ 1	13.3	26.79	
Lα 1	1.5	17.52	
Lβ 1	1.5	16.99	
Kα 1,2	11.9	70.69	
Kβ 1	13.3	62.39	

36	83.80		
Kr			
Krypton	0.003		
Kα 1,2	12.6	28.21	
Kα 1,2	12.6	40.32	
Kβ 1	14.1	25.20	
Lα 1	1.6	126.81	
Lβ 1	1.6	120.14	

46	106.42		
Pd			
Palladium	12.02		
Kα 1,2	21.2	16.71	
Kα 1,2	21.2	23.73	
Kβ 1	23.8	14.85	
Lα 1	2.8	59.95	
Lβ 1	3.0	56.63	
Kα 1,2	21.2	37.94	
Kβ 1	23.8	33.60	

47	107.87		
Ag			
Silver	10.55		
Kα 1,2	22.2	15.96	
Kα 1,2	22.2	22.66	
Kβ 1	24.9	14.18	
Lα 1	3.0	56.75	
Lβ 1	3.2	53.50	
Kα 1,2	22.2	36.19	
Kβ 1	24.9	32.04	

48	112.41		
Cd			
Cadmium	8.69		
Kα 1,2	23.1	15.27	
Kα 1,2	23.1	21.66	
Kβ 1	26.1	13.55	
Lα 1	3.1	53.82	
Lβ 1	3.3	50.63	
Kα 1,2	23.1	34.65	
Kβ 1	26.1	30.59	

49	114.82		
In			
Indium	7.31		
Kα 1,2	24.2	14.61	
Kα 1,2	24.2	20.72	
Kβ 1	27.3	12.96	
Lα 1	3.3	51.12	
Lβ 1	3.5	47.99	
Kα 1,2	24.2	33.04	
Kβ 1	27.3	29.24	

50	118.71		
Sn			
Tin	7.29		
Kα 1,2	25.2	13.99	
Kα 1,2	25.2	19.84	
Kβ 1	28.5	12.41	
Lα 1	3.4	48.64	
Lβ 1	3.7	45.56	
Kα 1,2	25.2	31.62	
Kβ 1	28.5	27.97	

51	121.76		
Sb			
Antimony	6.64		
Kα 1,2	26.4	13.41	
Kα 1,2	26.4	19.01	
Kβ 1	29.7	11.89	
Lα 1	3.6	46.34	
Lβ 1	3.8	43.31	
Kα 1,2	26.4	30.28	
Kβ 1	29.7	26.78	

52	127.60		
Te			
Tellurium	6.23		
Kα 1,2	27.4	12.87	
Kα 1,2	27.4	18.23	
Kβ 1	31.0	11.40	
Lα 1	3.8	44.20	
Lβ 1	4.0	41.21	
Kα 1,2	27.5	29.02	
Kβ 1	31.0	25.67	

53	126.90		
I			
Iodine	4.93		
Kα 1,2	28.6	12.35	
Kα 1,2	28.6	17.50	
Kβ 1	32.3	10.94	
Lα 1	3.9	42.22	
Lβ 1	4.2	39.27	
Kα 1,2	28.6	27.84	
Kβ 1	32.3	24.62	

54	131.29		
Xe			
Xenon	0.005		
Kα 1,2	29.7	11.85	
Kα 1,2	29.7	16.81	
Kβ 1	33.6	10.50	
Lα 1	4.1	40.37	
Lβ 1	4.4	37.42	

78	195.08		
Pt			
Platinum	21.46		
Lα 1	9.4	38.06	
Lβ 1	11.1	32.29	
Mα 1	2.0	87.53	
Lα 1	9.4	93.62	
Lβ 1	11.1	76.91	

79	196.97		
Au			
Gold	19.28		
Lα 1	9.7	36.96	
Lβ 1	11.4	31.22	
Mα 1	2.1	83.83	
Lα 1	9.7	90.27	
Lβ 1	11.4	73.98	

80	200.59		
Hg			
Mercury	13.53		
Lα 1	10.0	35.90	
Lβ 1	11.8	30.19	
Mα 1	2.1	80.49	
Lα 1	10.0	87.13	
Lβ 1	11.8	71.22	

81	204.37		
Tl			
Thallium	11.86		
Lα 1	10.3	34.92	
Lβ 1	12.2	29.20	
Mα 1	2.3	77.30	
Lα 1	10.3	84.20	
Lβ 1	12.2	68.62	

82	207.20		
Pb			
Lead	11.34		
Lα 1	10.6	33.93	
Lβ 1	12.6	28.25	
Mα 1	2.3	74.41	
Lα 1	10.6	81.45	
Lβ 1	12.6	66.15	

83	208.98		
Bi			
Bismuth	9.81		
Lα 1	10.8	33.00	
Lβ 1	13.0	27.34	
Mα 1	2.4	71.67	
Lα 1	10.8	78.86	
Lβ 1	13.0	63.82	

84	(209)		
Po			
Polonium	9.32		
Lα 1	11.1	32.11	
Lβ 1	13.4	26.47	
Lα 1	11.1	76.41	
Lβ 1	13.4	61.59	

85	(210)		
At			
Astatine	7.00		
Lα 1	11.4	31.26	
Lβ 1	13.9	25.64	

86	(222)		
Rn			
Radon	0.01		
Lα 1	11.7	30.44	
Lβ 1	14.3	24.84	

63	151.96		
Eu			
Europium	5.24		
Lα 1	5.9	96.23	
Lα 1	5.9	63.55	
Lβ 1	6.5	56.96	

64	157.25		
Gd			
Gadolinium	7.90		
Lα 1	6.1	91.87	
Lα 1	6.1	61.09	
Lβ 1	6.7	54.59	

65	158.93		
Tb			
Terbium	8.23		
Lα 1	6.3	87.87	
Lα 1	6.3	58.78	
Lβ 1	7.0	52.36	

66	162.50		
Dy			
Dysprosium	8.55		
Lα 1	6.5	84.15	
Lα 1	6.5	56.59	
Lβ 1	7.2	50.27	

67	164.93		
Ho			
Holmium	8.80		
Lα 1	6.7	80.73	
Lα 1	6.7	54.53	
Lβ 1	7.5	48.30	

68	167.26		
Er			
Erbium	9.07		
Lα 1	7.0	77.58	
Lα 1	7.0	52.60	
Lβ 1	7.8	46.43	

69	168.93		
Tm			
Thulium	9.32		
Lα 1	7.2	74.63	
Lα 1	7.2	50.78	
Lβ 1	8.1	44.67	

70	173.04		
Yb			
Ytterbium	6.97		
Lα 1	7.4	71.89	
Lα 1	7.4	49.06	
Lβ 1	8.4	42.99	
Lα 1	7.4	136.36	
Lβ 1	8.4	110.04	

71	174.47		
Lu			
Lutetium	9.84		
Lα 1	7.7	69.31	
Lα 1	7.7	47.42	
Lβ 1	8.7	41.40	
Lα 1	7.7	128.12	
Lβ 1	8.7	104.46	

95	(243)		
Am			
Americium	13.69		
Lα 1	14.6	34.65	
Lα 1	14.6	24.32	
Lβ 1	18.8	18.81	

96	(247)		
Cm			
Curium	13.51		
Lα 1	15.0	33.84	
Lα 1	15.0	23.76	
Lβ 1	19.4	18.26	

97	(247)		
Bk			
Berkelium	14.79		
Lα 1	15.3	33.04	
Lα 1	15.3	23.20	
Lβ 1	20.0	17.74	

98	(251)		
Cf			
Californium	15.1		
Lα 1	15.7	32.38	
Lα 1	15.7	22.68	
Lβ 1	20.6	17.22	

99	(252)		
Es			
Einsteinium	13.5		

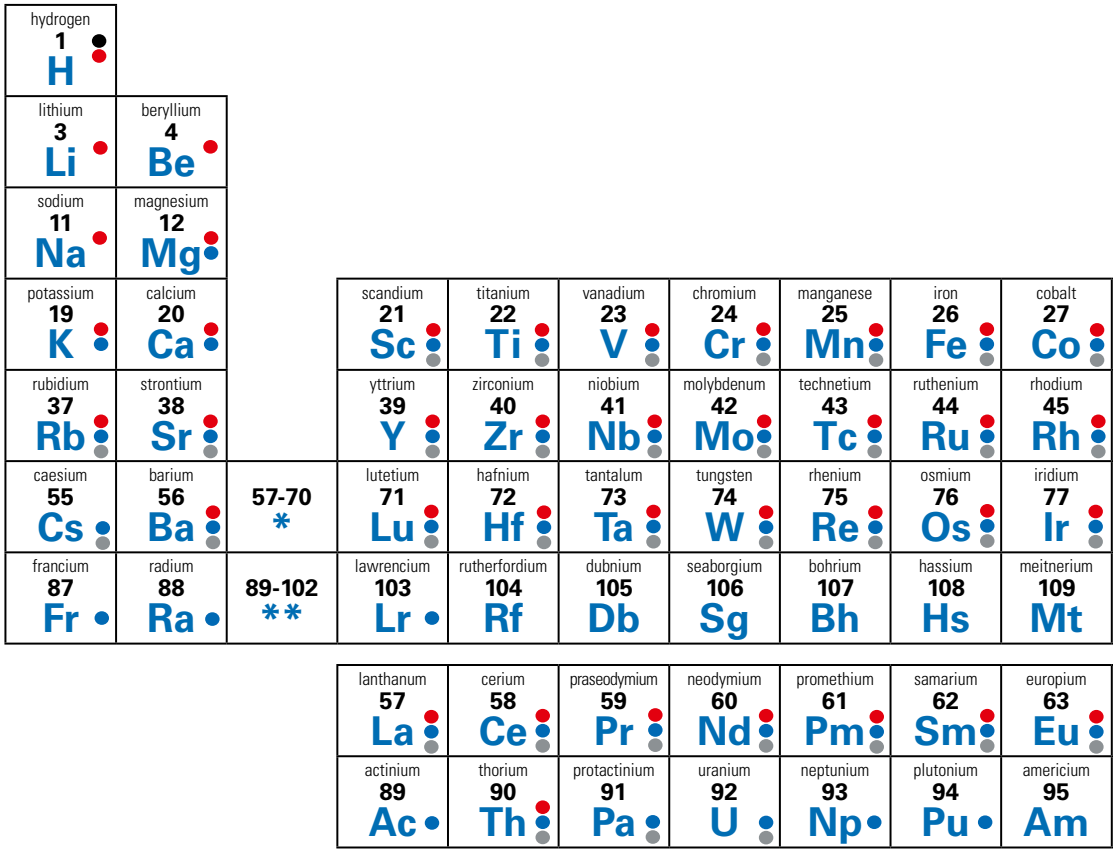
100	(257)		
Fm			
Fermium			

101	(258)		
Md			
Mendelevium			

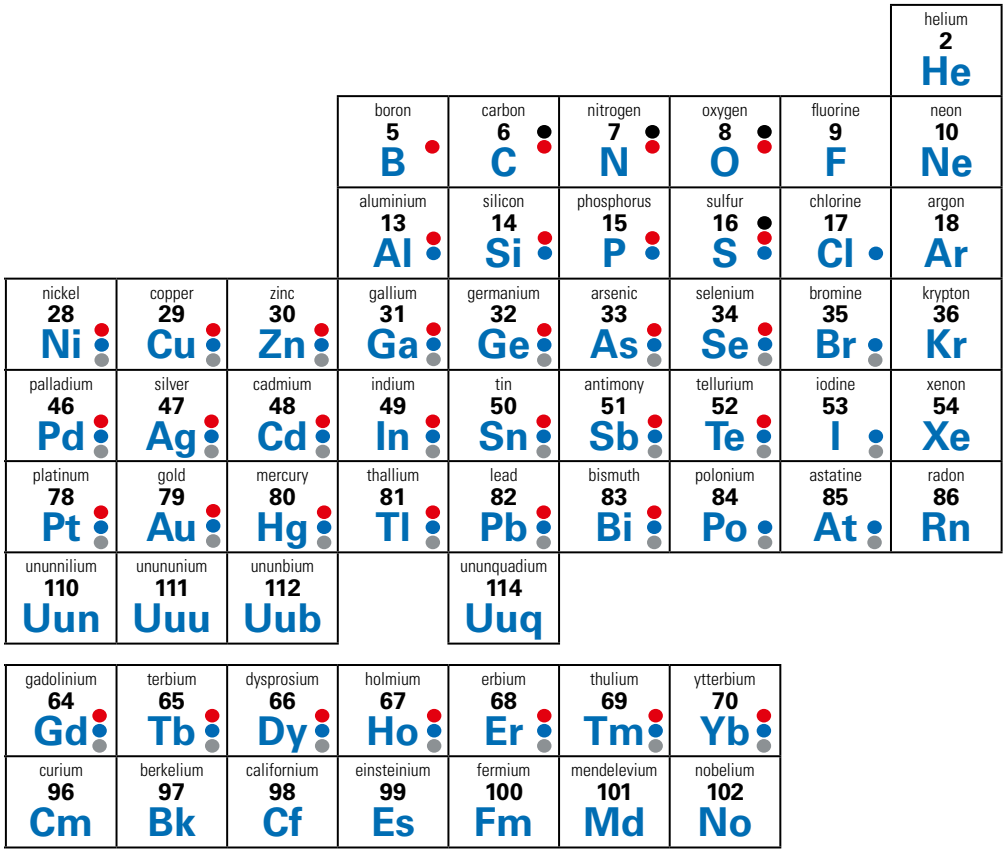
102	(259)		
No			
Nobelium			

103	(262)		
Lr			
Lawrencium			

Our Portfolio for Elemental Analysis



- Spark Spectrometers
- CS/ONH-Analyzers



Handheld XRF-Analyzers

μ-XRF Spectrometers

Spectral Lines used for OES

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Ag	230,9644	231,0354	I
Ag	235,7920	235,8641	II
Ag	241,3184	241,3918	II
Ag	328,0683	328,1628	I
Ag	338,2890	338,3861	I
Al	256,7987	256,8757	I
Al	266,0386	266,1178	I
Al	305,9933	306,0823	I
Al	308,2153	308,3048	I
Al	394,4006	394,5122	I
Al	396,1520	396,2641	I
As	188,9789	189,0420	I
As	234,9840	235,0559	I
As	289,8710	289,9560	I
Au	242,7950	242,8687	I
Au	264,1480	264,2267	I
Au	267,5950	267,6745	I
B	182,5786	182,6410	I
B	208,9590	209,0255	I
B	249,6770	249,7523	I
B	345,1410	345,2399	II
Ba	455,4042	455,5319	II
Be	234,8610	234,9329	I
Be	298,6090	298,6910	I
Be	301,9330	302,0210	I
Be	313,0420	313,1327	II
Bi	306,7720	306,8612	I
Bi	351,0850	351,1854	I
C	133,5207	133,5708	II
C	165,7478	165,8122	I
C	193,0268	193,0905	I
Ca	393,3664	393,4778	II
Ca	396,8470	396,9593	II
Ca	422,6730	422,7920	I
Ca	443,4960	443,6205	I
Cd	214,4410	214,5085	II
Cd	228,8022	228,8728	I
Cd	308,0827	308,1722	II
Cd	346,6200	346,7193	I
Cd	361,0508	361,1538	I
Cd	467,8149	467,9458	I
Ce	399,9240	400,0371	II
Ce	401,2390	401,3524	II
Ce	413,7646	413,8813	II
Ce	418,6600	418,7780	II
Ce	446,0210	446,1462	II
Co	228,6156	228,6861	II
Co	258,0320	258,1093	II
Co	345,3505	345,4494	I
Cr	265,8590	265,9381	II
Cr	267,7160	267,7956	II

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Cr	286,2570	286,3411	II
Cr	298,9190	299,0062	II
Cr	425,4332	425,5529	I
Cu	200,0348	200,0996	II
Cu	224,2618	224,3314	II
Cu	296,1160	296,2025	I
Cu	324,7540	324,8477	I
Cu	327,3960	327,4904	I
Cu	453,0819	453,2089	I
Cu	510,5540	510,6963	I
Fe	187,6710	187,7340	II
Fe	249,3260	249,4012	II
Fe	259,9400	260,0177	II
Fe	271,4410	271,5215	II
Fe	273,0730	273,1538	II
Fe	281,3287	281,4116	I
Fe	360,8859	360,9888	I
Fe	371,9935	372,0993	I
Fe	238,2040	238,2767	II
Ga	417,2040	417,3216	I
Ge	303,9067	303,9951	I
H	121,5144	121,5668	I
Hf	277,3360	277,4179	II
Hg	253,6520	253,7282	I
Hg	435,8350	435,9575	I
Hg	579,0660	579,2266	I
In	260,1760	260,2538	I
In	293,2630	293,3488	I
In	451,1323	451,2588	I
Ir	380,0120	380,1199	I
K	766,4900	766,7010	I
La	412,3230	412,4393	II
La	433,3753	433,4972	II
Li	497,1750	497,3137	I
Li	610,3650	610,5340	I
Mg	279,0790	279,1613	II
Mg	279,5530	279,6354	II
Mg	285,2130	285,2968	I
Mg	291,5450	291,6304	I
Mg	382,9350	383,0437	I
Mg	383,8290	383,9379	I
Mg	448,1130	448,2387	II
Mg	517,2699	517,4140	I
Mn	257,6100	257,6872	II
Mn	263,8170	263,8956	II
Mn	293,3060	293,3918	II
Mn	346,0330	346,1321	II
Mn	403,3073	403,4213	I
Mn	403,4490	403,5630	I
Mo	202,0300	202,0952	II
Mo	277,5400	277,6219	II

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Mo	281,6150	281,6979	II
Mo	290,9120	290,9972	II
Mo	308,7620	308,8517	II
Mo	386,4110	386,5206	I
N	149,2192	149,2625	I
N	174,4631	174,5252	I
Na	588,9950	589,1583	I
Na	589,5920	589,7558	I
Nb	210,9420	211,0089	II
Nb	313,0790	313,1698	II
Nb	319,4980	319,5904	II
Nb	410,0400	410,1557	I
Nb	410,0920	410,2078	I
Nb	416,4660	416,5834	I
Nd	410,9460	411,0620	II
Ni	218,5500	218,6184	II
Ni	225,3850	225,4548	II
Ni	231,6040	231,6752	II
Ni	243,7890	243,8629	II
Ni	341,4760	341,5740	I
Ni	351,5054	351,6059	I
Ni	352,4540	352,5548	I
Ni	361,9392	362,0424	I
Ni	376,9455	377,0526	I
Ni	471,4420	471,5739	I
Ni	490,4413	490,5783	I
O	130,1661	130,2168	I
P	178,2249	178,2870	I
P	253,5650	253,6412	I
P	255,3262	255,4028	I
Pb	220,3505	220,4193	II
Pb	283,3052	283,3885	I
Pb	322,0538	322,1468	I
Pb	405,7820	405,8966	I
Pb	416,8033	416,9208	I
Pd	324,2700	324,3635	I
Pd	340,4580	340,5557	I
Pd	360,9550	361,0580	I
Pr	418,9480	419,0661	II
Pt	265,9450	266,0241	I
Pt	270,5890	270,6692	I
Pt	299,7970	299,8844	I
Rh	343,4890	343,5875	I
Ru	349,8940	349,9941	I
S	180,6688	180,7311	I
Sb	206,8341	206,9001	I
Sb	217,5810	217,6492	I
Sb	231,1470	231,2181	I
Sb	259,8050	259,8827	I
Sb	276,9950	277,0768	I
Sb	287,7920	287,8764	I

Element	Lambda Air [nm]	Lambda Vacuum [nm]	Type I Atom II ION
Sb	326,7510	326,8452	I
Sc	361,3840	361,4871	II
Se	196,0259	196,0901	I
Si	212,4150	212,4821	I
Si	251,6123	251,6880	I
Si	288,1595	288,2440	I
Si	390,5523	390,6629	I
Sm	443,4320	443,5565	II
Sn	189,9278	189,9910	II
Sn	266,1248	266,2040	I
Sn	276,1780	276,2596	I
Sn	283,9990	284,0825	I
Sn	317,5050	317,5969	I
Sr	460,7330	460,8621	I
Sr	487,2490	487,3851	I
Ta	240,0630	240,1361	I
Ta	331,1160	331,2113	I
Te	169,9536	170,0000	I
Te	185,6573	185,7200	I
Te	214,2750	214,3425	I
Te	238,5780	238,6508	I
Th	401,9129	402,0265	II
Ti	311,2050	311,2953	II
Ti	324,1990	324,2926	II
Ti	337,2800	337,3769	II
Ti	365,3500	365,4541	I
Ti	367,1670	367,2716	I
Ti	368,5200	368,6249	II
Ti	498,1730	498,3120	I
Tl	351,9240	352,0246	I
Tl	377,5720	377,6792	I
V	214,0087	214,0761	II
V	288,2500	288,3345	II
V	311,0710	311,1612	II
V	369,2225	369,3276	I
V	437,9240	438,0471	I
W	209,8600	209,9266	II
W	220,4480	220,5168	II
W	400,8750	400,9883	I
Y	371,0300	371,1356	II
Y	464,3700	464,5000	II
Zn	206,1910	206,2569	II
Zn	213,8560	213,9234	I
Zn	250,2001	250,2755	II
Zn	334,5020	334,5982	I
Zn	481,0530	481,1875	I
Zr	332,6800	332,7757	II
Zr	343,8230	343,9216	II
Zr	349,6210	349,7210	II
Zr	357,2470	357,3490	II

X-ray Diffractometry Tables

Conversion from the 2Θ Bragg angle using Ag, Mo and Cu radiation to resolution and vice versa.

Calculations based on Bragg's Law: $2\,d \sin\Theta = n\,\lambda$

For λ, the mean of α_1 and α_2 $(2/3\,\alpha_1 + 1/3\,\alpha_2)$ was taken, resulting in following wavelengths:

Ag	0.56083 Å
Mo	0.71073 Å
Cu	1.54178 Å

$2\Theta_{Ag}$ (°)	$2\Theta_{Mo}$ (°)	$2\Theta_{Cu}$ (°)	d (Å)	sin Θ/λ	$2\Theta_{Ag}$ (°)	$2\Theta_{Mo}$ (°)		d (Å)	sin Θ/λ
3.21	4.07	8.84	**10.000**	0.050	**50.00**	64.77		0.664	0.754
3.63	4.61	**10.00**	8.845	0.057	53.32	69.30		0.625	**0.800**
6.43	8.15	17.74	**5.000**	**0.100**	53.82	**70.00**		0.620	0.807
7.24	9.18	**20.00**	4.439	0.113	**60.00**	78.64		0.561	0.892
7.89	**10.00**	21.80	4.077	0.123	60.96	**80.00**		0.553	0.904
10.00	12.68	27.73	3.217	0.155	67.83	**90.00**		0.503	0.995
10.73	13.61	29.78	**3.000**	0.167	68.23	90.59		**0.500**	**1.000**
10.80	13.70	**30.00**	2.979	0.168	**70.00**	93.25		0.489	1.023
12.88	16.34	35.92	2.500	**0.200**	74.38	**100.00**		0.464	1.078
14.29	18.14	**40.00**	2.254	0.222	**80.00**	109.09		0.436	1.146
15.75	**20.00**	44.26	2.046	0.244	80.54	**110.00**		0.434	1.153
16.12	20.47	45.34	**2.000**	0.250	84.60	117.05		0.417	**1.200**
17.69	22.47	**50.00**	1.824	0.274	86.22	**120.00**		0.410	1.219
19.37	24.62	55.10	1.667	**0.300**	89.02	125.35		**0.400**	1.250
20.00	25.43	57.03	1.615	0.310	**90.00**	127.30		0.397	1.261
20.96	26.65	**60.00**	1.542	0.324	91.31	**130.00**		0.392	1.275
21.55	27.41	61.85	**1.500**	0.333	95.72	**140.00**		0.378	1.322
23.57	**30.00**	68.31	1.373	0.364	99.32	**150.00**		0.368	1.359
24.09	30.66	**70.00**	1.344	0.372	**100.00**	152.24		0.366	1.366
25.93	33.03	76.15	1.250	**0.400**	101.99	**160.00**		0.361	1.386
27.04	34.47	**80.00**	1.199	0.417	103.47	168.56		0.357	**1.400**
29.81	38.05	**90.00**	1.090	0.459	103.64	**170.00**		0.357	1.402
30.00	38.29	90.72	1.083	0.461	104.20	**180.00**		0.355	1.407
31.31	**40.00**	95.80	1.039	0.481	**110.00**			0.342	1.461
32.36	41.36	**100.00**	1.006	0.497	**120.00**			0.324	1.544
32.57	41.63	100.87	**1.000**	**0.500**	127.62			0.313	**1.600**
34.67	44.37	**110.00**	0.941	0.531	**130.00**			0.309	1.616
36.72	47.06	**120.00**	0.890	0.562	138.36			**0.300**	1.667
38.50	49.39	**130.00**	0.851	0.588	**140.00**			0.298	1.676
38.96	**50.00**	132.92	0.841	0.595	**150.00**			0.290	1.722
39.33	50.48	135.36	0.833	**0.600**	**160.00**			0.285	1.756
39.97	51.34	**140.00**	0.820	0.609	**170.00**			0.281	1.776
40.00	51.37	140.19	0.820	0.610	**180.00**			0.280	1.783
41.04	52.75	149.00	**0.800**	0.625					
41.14	52.88	**150.00**	0.798	0.626					
41.98	54.00	**160.00**	0.783	0.639					
42.49	54.67	**170.00**	0.774	0.646					
42.66	54.90	**180.00**	0.771	0.649					
46.23	59.67		0.714	**0.700**					
46.48	**60.00**		0.711	0.704					
47.23	61.02		**0.700**	0.714					

EPR/ENDOR Frequency Table

Z	A	E	Spin I	Nat. Abund. [%] (Half-life)	calc. X-Band ENDOR Freq. [MHz at 0.350 T] (free nucleus)	$g = \mu / (I\ \mu_N)$	$g\ \mu_N / g_e\ \mu_B$	Quadrupole Moment Q [fm^2 = 0.01 barn]
0	1	n	1/2		10.2076432	–3.8260854	1.040669 E–03	
1	1 2 3	H H H	1/2 1 1/2	99.9885 0.0115 (12.32 y)	14.9021186 2.28756617 15.8951945	5.58569468 0.857438228 5.95792488	–1.519270 E–03 –2.332173 E–04 –1.620514 E–03	0.286
2	3	He	1/2	0.000134	11.3519357	–4.25499544	1.157329 E–03	
3	6 7	Li Li	1 3/2	7.59 92.41	2.193146 5.791961	0.8220473 2.1709750	–2.235912 E–04 –5.904902 E–04	–0.0808 –4.01
4	9	Be	3/2	100.0	2.09429	–0.784993	2.13513 E–04	5.288
5	10 11	B B	3 3/2	19.9 80.1	1.601318 4.782045	0.600214927 1.792433	–1.632543 E–04 –4.875293 E–04	8.459 4.059
6	13	C	1/2	1.07	3.747940	1.404824	–3.821023 E–04	
7	14 15	N N	1 1/2	99.636 0.364	1.077197 1.511043	0.40376100 –0.56637768	–1.098202 E–04 1.540508 E–04	2.044
8	17	O	5/2	0.038	2.02098	–0.757516	2.06039 E–04	–2.558
9	19	F	1/2	100.0	14.01648	5.253736	–1.428980 E–03	
10	21	Ne	3/2	0.27	1.177076	–0.441198	1.20003 E–04	10.155
11	22 23	Na Na	3 3/2	(2.6019 y) 100.0	1.5527 3.944334	0.5820 1.4784371	–1.583 E–04 –4.021247 E–04	 10.4
12	25	Mg	5/2	10.00	0.91290	–0.34218	9.3071 E–05	19.94
13	27	Al	5/2	100.0	3.886082	1.4566028	–3.961859 E–04	14.66
14	29	Si	1/2	4.685	2.96293	–1.11058	3.02070 E–04	
15	31	P	1/2	100.0	6.03801	2.26320	–6.15575 E–04	
16	33	S	3/2	0.75	1.145104	0.429214	–1.16743 E–04	–6.78
17	35 36 37	Cl Cl Cl	3/2 2 3/2	75.76 (3.01 E5 y) 24.24	1.461790 1.71476 1.216786	0.5479162 0.642735 0.4560824	–1.490294 E–04 –1.748195 E–04 –1.240513 E–04	–8.165 –1.80 –6.435
18	39	Ar	7/2	(269 y)	1.21	–0.454	1.234 E–04	
19	39 40 41	K K K	3/2 4 3/2	93.258 0.0117 6.730	0.696337 0.865803 0.382209	0.2610049 –0.324525 0.143261827	–7.099152 E–05 8.82686 E–05 –3.896623 E–05	5.85 –7.3 7.11
20	41 43	Ca Ca	7/2 7/2	(1.02 E5 y) 0.135	1.215637 1.004386	–0.4556517 –0.3764694	1.239341 E–04 1.023971 E–04	–6.7 –4.08
21	45	Sc	7/2	100.0	3.625677	1.358996	–3.696376 E–04	–22.0
22	47 49	Ti Ti	5/2 7/2	7.44 5.41	0.84144 0.84166	–0.31539 –0.315477	8.5784 E–05 8.58076 E–05	30.2 24.7
23	50 51	V V	6 7/2	0.250 99.750	1.487665 3.924649	0.5576148 1.4710588	–1.516674 E–04 –4.001178 E–04	21 –5.2
24	53	Cr	3/2	9.501	0.844019	–0.31636	8.6048 E–05	–15 or –2.8
25	53 55	Mn Mn	7/2 5/2	(3.74 E6 y) 100.0	3.8296 3.701688	1.4354 1.38748716	–3.9043 E–04 –3.773869 E–04	 33
26	57	Fe	1/2	2.119	0.483548	0.18124600	–4.92977 E–05	
27	59 60	Co Co	7/2 5	100.0 (1925 d)	3.527 2.027	1.322 0.7598	–3.596 E–04 –2.067 E–04	42 44
28	61	Ni	3/2	1.1399	1.33399	–0.50001	1.3600 E–04	16.2
29	63 65	Cu Cu	3/2 3/2	69.15 30.85	3.961568 4.2359	1.484897 1.5877	–4.038817 E–04 –4.318525 E–04	–22.0 –20.4
30	67	Zn	5/2	4.102	0.933986	0.35008196	–9.521988 E–05	15
31	69 71	Ga Ga	3/2 3/2	60.108 39.892	3.58672 4.55726	1.34439 1.70818	–3.6567 E–04 –4.6461 E–04	17.1 10.7
32	73	Ge	9/2	7.76	0.521409	–0.1954373	5.315759 E–05	–19.6
33	75	As	3/2	100.0	2.56025	0.959647	–2.61017 E–04	31.4
34	77 79	Se Se	1/2 7/2	7.63 (2.95 E5 y)	2.855058 0.7760	1.0701486 –0.2909	–2.910730 E–04 7.911 E–05	 80
35	79 81	Br Br	3/2 3/2	50.69 49.31	3.746454 4.038433	1.404267 1.513708	–3.819508 E–04 –4.117181 E–04	30.5 25.4
36	83 85	Kr Kr	9/2 9/2	11.500 (10.756 y)	0.575479 0.596	–0.215704 –0.2233	5.86701 E–05 6.075 E–05	25.9 43.3
37	85 87	Rb Rb	5/2 3/2	72.17 27.83	1.444247 4.894398	0.5413406 1.834545	–1.472409 E–04 –4.989836 E–04	27.6 13.35
38	87	Sr	9/2	7.00	0.648363	–0.243023	6.61005 E–05	33.5
39	89	Y	1/2	100.0	0.733223	–0.2748308	7.475208 E–05	

EPR/ENDOR Frequency Table

Z	A	E	Spin I	Nat. Abund. [%] (Half-life)	calc. X-Band ENDOR Freq. [MHz at 0.350 T] (free nucleus)	$g = \mu / (I\ \mu_N)$	$g\ \mu_N / g_e\ \mu_B$	Quadrupole Moment Q [fm^2 = 0.01 barn]
40	91	Zr	5/2	11.22	1.39118	–0.521448	1.41830 E–04	–17.6
41	93	Nb	9/2	100.0	3.6583	1.37122	–3.72963 E–04	–32
42	95 97	Mo Mo	5/2 5/2	15.90 9.56	0.9756 0.9962	–0.3657 –0.3734	9.9462 E–05 1.016 E–04	–2.2 25.5
43	99	Tc	9/2	(2.1 E5 y)	3.3703	1.2633	–3.4360 E–04	–12.9
44	99 101	Ru Ru	5/2 5/2	12.76 17.06	0.684 0.764	–0.256 –0.286	6.97 E–05 7.79 E–05	7.9 45.7
45	103 105	Rh Rh	1/2 7/2	100.0 (35.36 h)	0.47169 3.39	–0.17680 1.27	4.8088 E–05 –3.46 E–04	
46	105	Pd	5/2	22.33	0.685	–0.257	6.98 E–05	66
47	107 109	Ag Ag	1/2 1/2	51.839 48.161	0.606574 0.69734	–0.2273593 –0.26138	6.184016 E–05 7.1094 E–05	
48	111 113	Cd Cd	1/2 1/2	12.80 12.22	3.174203 3.320483	–1.1897722 –1.2446018	3.236098 E–04 3.385231 E–04	
49	113 115	In In	9/2 9/2	4.29 95.71	3.2779 3.2850	1.2286 1.2313	–3.3418 E–04 –3.3490 E–04	79.9 81
50	115 117 119	Sn Sn Sn	1/2 1/2 1/2	0.34 7.68 8.59	4.9027 5.34136 5.5881	–1.8377 –2.00208 –2.09456	4.9983 E–04 5.44552 E–04 5.69706 E–04	
51	121 123 125	Sb Sb Sb	5/2 7/2 7/2	57.21 42.79 (2.75856 y)	3.5893 1.9436 2.00	1.34536 0.72851 0.75	–3.65929 E–04 –1.9815 E–04 –2.04 E–04	–36 or –45 –49
52	123 125	Te Te	1/2 1/2	0.89 7.07	3.932218 4.740899	–1.4738956 –1.7770102	4.008894 E–04 4.833345 E–04	
53	127 129	I I	5/2 7/2	100.0 (1.57 E7 y)	3.00222 1.9979	1.125308 0.7489	–3.060760 E–04 –2.0368 E–04	–71 –48
54	129 131	Xe Xe	1/2 3/2	26.4006 21.2324	4.15114 1.230549	–1.555952 0.461241	4.232082 E–04 –1.254545 E–04	–11.4
55	133 134 135 137	Cs Cs Cs Cs	7/2 4 7/2 7/2	100.0 (2.0652 y) (2.3 E6 y) (30.07 y)	1.968173 1.9967 2.0828 2.163	0.7377214 0.74843 0.78069 0.8109	–2.006551 E–04 –2.0357 E–04 –2.12341 E–04 –2.205 E–04	–0.343 38.9 5.0 5.1
56	133 135 137	Ba Ba Ba	1/2 3/2 3/2	(10.51 y) 6.592 11.232	4.11749 1.491586 1.66716	–1.54334 0.559085 0.62489	4.19778 E–04 –1.520672 E–04 –1.69967 E–04	 16.0 24.5
57	137 138 139	La La La	7/2 5 7/2	(6 E4 y) 0.090 99.910	2.054 1.981533 2.121403	0.7700 0.7427292 0.7951559	–2.094 E–04 –2.020172 E–04 –2.1627690 E–04	26 45 20
59	141	Pr	5/2	100.0	4.5625	1.71016	–4.65152 E–04	–5.89
60	143 145	Nd Nd	7/2 7/2	12.2 8.3	0.8118 0.5000	–0.3043 –0.1874	8.2764 E–05 5.0979 E–05	–63 –33
61	147	Pm	7/2	(2.623 y)	1.97	0.737	–2.00 E–04	74
62	147 149 151	Sm Sm Sm	7/2 7/2 5/2	14.99 13.82 (90 y)	0.6211 0.5120 0.3874	–0.2328 –0.1919 –0.1452	6.332 E–05 5.220 E–05 3.949 E–05	–25.9 7.5 71
63	151 152 153 154 155	Eu Eu Eu Eu Eu	5/2 3 5/2 3 5/2	47.81 (13.537 y) 52.19 (8.593 y) (4.753 y)	3.70487 1.7253 1.6353 1.783 1.62	1.38868 0.6467 0.6130 –0.6683 0.608	–3.77711 E–04 –1.759 E–04 –1.667 E–04 1.818 E–04 –1.65 E–04	90.3 271 241 280 240
64	155 157	Gd Gd	3/2 3/2	14.80 15.65	0.4575 0.5999	–0.1715 –0.2249	4.664 E–05 6.116 E–05	127 135
65	157 158 159	Tb Tb Tb	3/2 3 3/2	(71 y) (180 y) 100.0	3.57 1.563 3.5821	1.34 0.5860 1.3427	–3.64 E–04 –1.594 E–04 –3.6520 E–04	141 270 143.2
66	161 163	Dy Dy	5/2 5/2	18.889 24.896	0.512 0.718	–0.192 0.269	5.22 E–05 –7.32 E–05	251 265
67	165	Ho	7/2	100.0	3.150	1.181	–3.211 E–04	358
68	167	Er	7/2	22.869	0.4298	–0.1611	4.382 E–05	357
69	169 171	Tm Tm	1/2 1/2	100.0 (1.92 y)	1.23 1.22	–0.462 –0.456	1.257 E–04 1.240 E–04	
70	171 173	Yb Yb	1/2 5/2	14.28 16.13	2.6341 0.72555	0.98734 –0.27196	–2.6855 E–04 7.3970 E–05	280

EPR/ENDOR Frequency Table

Z	A	E	Spin I	Nat. Abund. [%] (Half-life)	calc. X-Band ENDOR Freq. [MHz at 0.350 T] (free nucleus)	$g = \mu / (I\ \mu_N)$	$g\ \mu_N / g_e\ \mu_B$	Quadrupole Moment Q [fm^2 = 0.01 barn]
71	173	Lu	7/2	(1.37 y)	1.74	0.651	–1.772 E–04	
	174	Lu	1	(3.31 y)	5.1	1.9	–5.2 E–04	
	175	Lu	7/2	97.41	1.7016	0.6378	–1.735 E–04	349
	176	Lu	7	2.59	1.208	0.4527	–1.231 E–04	497
72	177	Hf	7/2	18.60	0.6049	0.2267	–6.166 E–05	337
	179	Hf	9/2	13.62	0.380	–0.142	3.87 E–05	379
73	181	Ta	7/2	99.988	1.8069	0.67729	–1.8422 E–04	317
74	183	W	1/2	14.31	0.628478	0.2355695	–6.407328 E–05	
75	185	Re	5/2	37.40	3.4012	1.2748	–3.4675 E–04	218
	187	Re	5/2	62.60	3.4359	1.2879	–3.5029 E–04	207
76	187	Os	1/2	1.96	0.344971	0.12930378	–3.516974 E–05	
	189	Os	3/2	16.15	1.173760	0.439955	–1.196648 E–04	85.6
77	191	Ir	3/2	37.3	0.26804	0.10047	–2.7326 E–05	81.6
	193	Ir	3/2	62.7	0.2912	0.1091	–2.9684 E–05	75.1
78	195	Pt	1/2	33.832	3.25229	1.21904	–3.31570 E–04	
79	197	Au	3/2	100.0	0.26351	0.098772	–2.6865 E–05	54.7
80	199	Hg	1/2	16.87	2.699312	1.011771	–2.751947 E–04	
	201	Hg	3/2	13.18	0.996420	–0.3734838	1.015850 E–04	38.6
81	203	Tl	1/2	29.52	8.656069	3.24451580	–8.824859 E–04	
	204	Tl	2	(3.78 y)	0.12	0.045	–1.22 E–05	
	205	Tl	1/2	70.48	8.741211	3.2764292	–8.911661 E–04	
82	207	Pb	1/2	22.1	3.1065	1.1644	–3.1670 E–04	
83	207	Bi	9/2	(32.9 y)	2.419	0.9069	–2.4667 E–04	–58
	209	Bi	9/2	100.0	2.437	0.9134	–2.4844 E–04	–51.6
84	209	Po	1/2	(102 y)	3.63	1.36	–3.70 E–04	
86	211	Rn	1/2	(14.6 h)	3.207	1.202	–3.269 E–04	
87	212	Fr	5	(20 min)	2.47	0.924	–2.51 E–04	–10
88	225	Ra	1/2	(14.9 d)	3.916	–1.468	3.993 E–04	
89	227	Ac	3/2	(21.77 y)	2.0	0.73	–1.99 E–04	170
90	229	Th	5/2	(7.34 E3 y)	0.491	0.184	–5.00 E–05	430
91	231	Pa	3/2	100.0 (3.25 E4 y)	3.57	1.34	–3.64 E–04	–172
92	233	U	5/2	(1.592 E5 y)	0.630	0.236	–6.42 E–05	366.3
	235	U	7/2	0.7204 (7.04 E8 y)	0.290	–0.109	2.95 E–05	493.6
93	237	Np	5/2	(2.14 E6 y)	3.351	1.256	–3.416 E–04	386.6
94	239	Pu	1/2	(2.410 E4 y)	1.08	0.406	–1.104 E–04	
	241	Pu	5/2	(14.4 y)	0.726	–0.272	7.40 E–05	560
95	241	Am	5/2	(432.7 y)	1.69	0.632	–1.72 E–04	314
	243	Am	5/2	(7.37 E3 y)	1.60	0.60	–1.63 E–04	286
96	243	Cm	5/2	(29.1 y)	0.438	0.164	–4.46 E–05	
	245	Cm	7/2	(8.48 E3 y)	0.38	0.14	–3.89 E–05	
	247	Cm	9/2	(1.56 E7 y)	0.22	0.082	–2.24 E–05	
97	249	Bk	3.5	(320 d)	1.5	0.6	–1.6 E–04	
99	253	Es	3.5	(20.47 d)	3.13	1.17	–3.19 E–04	670

revision 2009 based on NMR Properties Table, W. E. Hull; no. of decimal places reflects precision.

EPR Tables

Useful Relationships for EPR

Magn. Moment of the electron $\mu_e = g_e\ \mu_B\ S = g_e\ \mu_B / 2$ (g_e defined as negative) alternatively: $\mu_e = -g_e\ \mu_B / 2$ (with g_e positive) $\mu_B = \beta_e$ = Bohr magneton	**Magn. Moment for nucleus n** with spin I_n $\mu_n = g_n\ \mu_N\ I_n = \gamma_n\ \eta\ I_n$ $\mu_N = \beta_N$ = nuclear magneton
Resonance Condition - EPR $\nu_e = \|g\|\ \mu_B\ B_0 / h$ ν_e [GHz] = 13.996246 $\|g\|\ B_0$ [T] B_0 [T] = 0.071447730 ν_e [GHz] / $\|g\|$ $\|g\|$ = 0.071447730 ν_e [GHz] / B_0 [T] $\|g\|$ = 3.04198626 ν_e [GHz] / ν_{H2O} [MHz]	**Resonance Condition - NMR** $\nu_n = \|g_n\|\ \mu_N\ B_0 / h = \|\gamma_n\| B_0 / 2\pi$ for ^{1}H: ν_{H2O} [MHz] = 42.5763875 B_0 [T] B_0 [T] = 0.0234871970 ν_{H2O} [MHz]
Hyperfine Coupling A [MHz] = 2.99792458 $\times 10^4$ A [cm^{-1}] = 13.996246 $\|g\|$ A [mT] = 1.3996246 $\|g\|$ A [G]	A [cm^{-1}] = 0.333564095 $\times$ 10^{-4} A [MHz] = 4.6686451 $\times$ 10^{-4} $\|g\|$ A [mT] = 0.46686451 $\times$ 10^{-4} $\|g\|$ A [G]
Magnetic Field (flux density) = B_0 [in Tesla]	1 T = 10^4 G = 10 kG; 1 mT = 10 G; 1 G = 0.1 mT

see Physical Tables for Fundamental Constants

Skin Depth Table

Material	Specific Resistivity x 10^{-6} ohm-cm	Depth at 9.6 GHz		Depth at 100 kHz	
		μm	μin	mm	in
Silver	1.629	0.656	25.8	0.203	0.008
Copper. annealed	1.724	0.674	26.6	0.209	0.008
Gold	2.440	0.802	31.6	0.249	0.010
Aluminum	2.824	0.863	34.0	0.267	0.011
Rhodium	5.040	1.153	45.4	0.357	0.014
Tungsten	5.600	1.216	47.9	0.377	0.015
Molybdenum	5.700	1.226	48.3	0.380	0.015
Zinc	5.800	1.237	48.7	0.383	0.015
Brass	ca. 7.	1.359	53.5	0.421	0.017
Cadmium	7.600	1.416	55.8	0.439	0.017
Nickel	7.800	1.435	56.5	0.444	0.017
Platinum	10.000	1.624	64.0	0.503	0.020
Palladium	11.0	1.704	67.1	0.528	0.021
Tin	11.5	1.742	68.6	0.540	0.021
Lead	22.0	2.409	94.9	0.747	0.029

EPR Tables

Table for Various Free Radicals Generated in Aqueous Solution

Radical	Sample solution	T (°C) *p*H	T_1 (µs)	Radical	Sample solution	T (°C) *p*H	T_1 (µs)
$^{\bullet}CH_3$	0.1-0.5 M DMSO 1.0 M NaOH	19 *p*H = 14	0.2	$^{\bullet}CH_2OH$	0.5-1.0 M CH_3OH 1.0 M phosphate buffer	17 *p*H = 6.6-6.8	0.6
$^{\bullet}CH_2COO^-$	0.5 M NaOAc 1.0 M NaOH	17-19 *p*H = 14	2.0	$CH_3C^{\bullet}HOH$	0.5 M CH_3CH_2OH 1.0 M phosphate buffer	18 *p*H = 6.6-6.8	1.3
$^{\bullet}CH(COO^-)_2$	0.5 M malonic acid 2.0 M NaOH	18 *p*H = 14	2.9	$(CH_3)_2C^{\bullet}OH$	0.25 M *i*-propanol 0.5 M phosphate buffer	17 *p*H = 6.8	2.7
$^-OC^{\bullet}(COO^-)_2$	0.1 M tartronic acid 1.2 M NaOH	17 *p*H = 14	3.6 $3.5 \le T_1 < 4.0$	CH_2OD	0.5 M CH_3OH in D_2O acidif with H_2SO_4	9 *p*D = 3.6 19 *p*D = 3.2	0.72 0.53
$^-OCH^{\bullet}COO^-$	0.1 M tartronic acid 1.2 M NaOH	17 *p*H = 14	1.4				
$^{\bullet}CH_2O^-$	0.5 M CH_3OH 0.1 M NaOH	10 *p*H = 13	~0.1 $0.08 \le T_1 < 0.15$	$(CH_3)_2C^{\bullet}OD$	0.5 M *i*-propanol in D_2O acidif with H_2SO_4	19 *p*D = 3.5	2.2
$^{\bullet}CH_3C^{\bullet}OH$	0.5 M CH_3CH_2OH 1.0 M NaOH	18 *p*H = 14	0.7		0.5 M isopropanol in D_2O; 0.5 M phosphate buffer	19 *p*D = 7.0	2.5
$(CH_3)_2CO^{\bullet-}$	0.5 M *i*-propanol 1.0 M NaOH	16 *p*H = 14	1.6				

Relaxation Times of Some Organic Free Radicals (Saturation-Recovery Method)

Radical	T_1 (µs)	T_2 (µs)
1,2-dicarboxylvinyl	9.0±1	7.0±2
chelidonic acid trianion	5.0±0.5	4.5±1
ascorbate radical	2.3±0.5	1.0±0.3
p-benzosemiquinone anion	2.0±0.3	1.8±0.5
2,5-di-*t*-butyl-benzosemiquinone anion	11.5±0.5	. . .

Values of T_2 for Various Organic Radicals at 77 K (ESE Method)

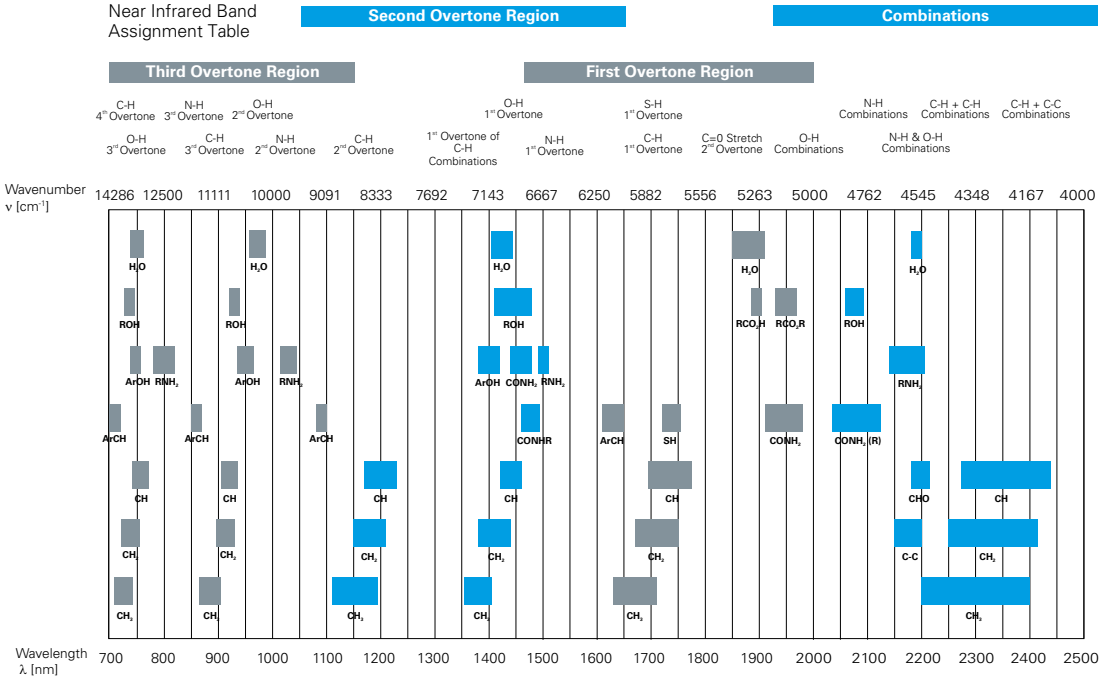
Radical	Matrix	T_2 (µs)
naphthalene anion	MTHF	3.4
naphtalene-d_8 anion	MTHF	3.2
1.3,5-triphenylbenzene anion	MTHF	3.2
triphenylene anion	MTHF	3.2
DPPH	MTHF	3.2
DPPH	fluorolube (FS-5)	10.0
perylene cation	sulfuric acid	10.4
anthracene cation	sulfuric acid	10.4
naphthacene cation	sulfuric acid	10.4
thianthrene cation	sulfuric acid	10.0
anthracene-d_{10} cation	sulfuric acid-d_2	200.0
anthracene cation	boric acid	14.6
biphenyl cation	boric acid	14.6
p-terphenyl cation	boric acid	14.2
naphthalene cation	boric acid	13.2
1,3,5-triphenylbenzene cation	boric acid	13.8
coronene cation	boric acid	10.0
triphenylene cation	boric acid	9.8
thianthrene cation	boric acid	10.0

IR Spectroscopy Tables

Conversion Table for Transmittance and Absorbance Units

Transmittance [%]	Absorbance	Transmittance [%]	Absorbance	Transmittance [%]	Absorbance	Transmittance [%]	Absorbance
1.0	2.000	26.0	.585	51.0	.292	76.0	.119
2.0	1.699	27.0	.569	52.0	.284	77.0	.114
3.0	1.523	28.0	.553	53.0	.276	78.0	.108
4.0	1.398	29.0	.538	54.0	.268	79.0	.102
5.0	1.301	30.0	.523	55.0	.260	80.0	.097
6.0	1.222	31.0	.509	56.0	.265	81.0	.092
7.0	1.155	32.0	.495	57.0	.244	82.0	.086
8.0	1.097	33.0	.481	58.0	.237	83.0	.081
9.0	1.046	34.0	.469	59.0	.229	84.0	.076
10.0	1.000	35.0	.456	60.0	.222	85.0	.071
11.0	.959	36.0	.444	61.0	.215	86.0	.066
12.0	.921	37.0	.432	62.0	.208	87.0	.060
13.0	.886	38.0	.420	63.0	.201	88.0	.056
14.0	.854	39.0	.409	64.0	.194	89.0	.051
15.0	.824	40.0	.398	65.0	.187	90.0	.046
16.0	.796	41.0	.387	66.0	.180	91.0	.041
17.0	.770	42.0	.377	67.0	.174	92.0	.036
18.0	.745	43.0	.367	68.0	.167	93.0	.032
19.0	.721	44.0	.357	69.0	.161	94.0	.027
20.0	.699	45.0	.347	70.0	.155	95.0	.022
21.0	.678	46.0	.337	71.0	.149	96.0	.018
22.0	.658	47.0	.328	72.0	.143	97.0	.013
23.0	.638	48.0	.319	73.0	.137	98.0	.009
24.0	.620	49.0	.310	74.0	.131	99.0	.004
25.0	.602	50.0	.301	75.0	.125	100.0	.000

Near-Infrared Table



IR Spectroscopy Tables

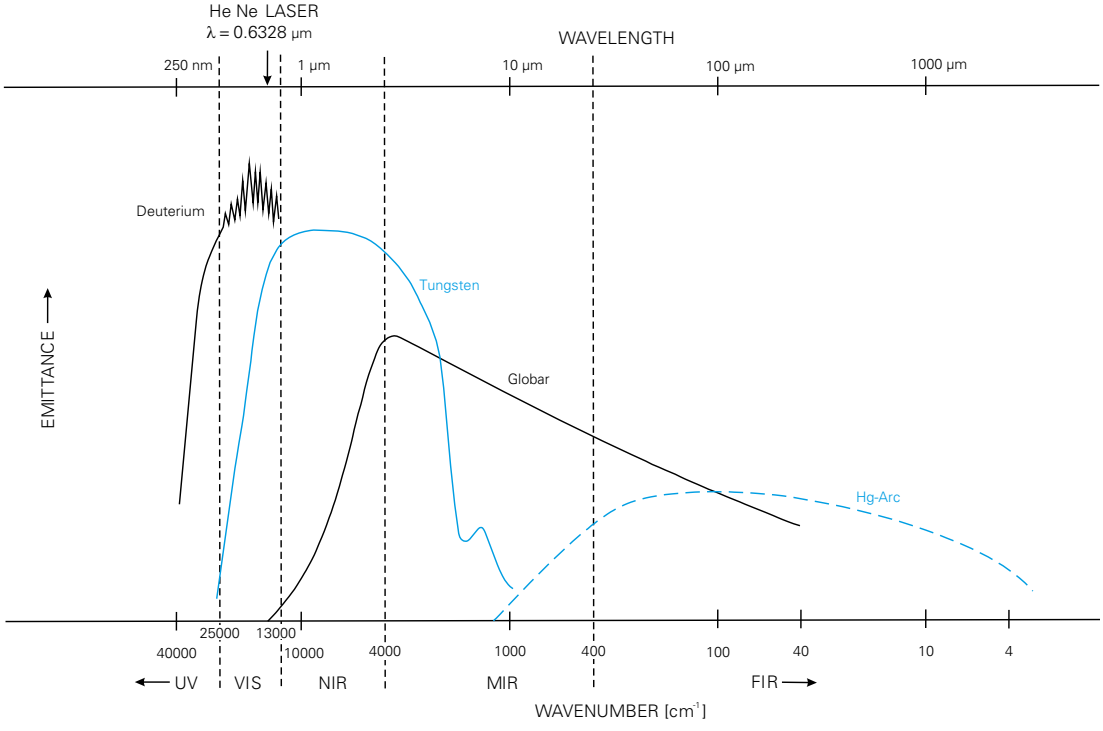
Conversion Table for Energy and Wavelength Units

Wavenumber [cm^{-1}]	Wavelength [μm]	Wavelength [nm]	Frequency [GHz]	Electron Volt [eV]
2.0	5 000.00	5 000 000	60	.00 025
4.0	2 500.00	2 500 000	120	.00 050
6.0	1 666.67	1 666 667	180	.00 074
8.0	1 250.00	1 250 000	240	.00 099
10.0	1 000.00	1 000 000	300	.00 124
12.0	833.33	833 333	360	.00 149
14.0	714.29	714 286	420	.00 174
16.0	625.00	625 000	480	.00 198
18.0	555.56	555 556	540	.00 223
20.0	500.00	500 000	600	.00 248
22.0	454.55	454 545	660	.00 273
24.0	416.57	416 667	719	.00 298
26.0	384.62	384 615	779	.00 322
28.0	357.14	357 143	839	.00 347
30.0	333.33	333 333	898	.00 372
32.0	312.50	312 500	959	.00 397
34.0	294.12	294 118	1 019	.00 422
36.0	277.78	277 778	1 079	.00 446
38.0	263.16	263 158	1 139	.00 471
40.0	250.00	250 000	1 199	.00 496
50.0	200.00	200 000	1 499	.00 620
60.0	166.67	166 667	1 799	.00 744
70.0	142.86	142 857	2 099	.00 868
80.0	125.00	125 000	2 398	.00 992
90.0	111.11	111 111	2 698	.01 116
100.0	100.00	100 000	2 988	.01 240
110.0	90.91	90 909	3 298	.01 364
120.0	83.33	83 333	3 597	.01 488
130.0	76.92	76 923	3 897	.01 612
140.0	71.43	71 429	4 197	.01 736
150.0	66.67	66 667	4 497	.01 860
160.0	62.50	62 500	4 797	.01 984
170.0	58.82	58 824	5 096	.02 108
180.0	55.56	55 556	5 396	.02 232
190.0	52.63	52 632	5 696	.02 356
200.0	50.00	50 000	5 996	.02 480
220.0	45.45	45 455	6 595	.02 728
240.0	41.67	41 667	7 195	.02 976
260.0	38.46	38 462	7 795	.03 224
280.0	35.71	35 714	8 394	.03 472
300.0	33.33	33 333	8 994	.03 720
320.0	31.25	31 250	9 593	.03 967
340.0	29.41	29 412	10 193	.04 215
360.0	27.78	27 778	10 792	.04 463
380.0	26.32	26 316	11 329	.04 711
400.0	25.00	25 000	11 992	.04 959
500.0	20.00	20 000	14 990	.06 199
600.0	16.67	16 667	17 987	.07 439
700.0	14.29	14 286	20 985	.08 679
800.0	12.50	12 500	23 983	.09 919
900.0	11.11	11 111	26 981	.11 159

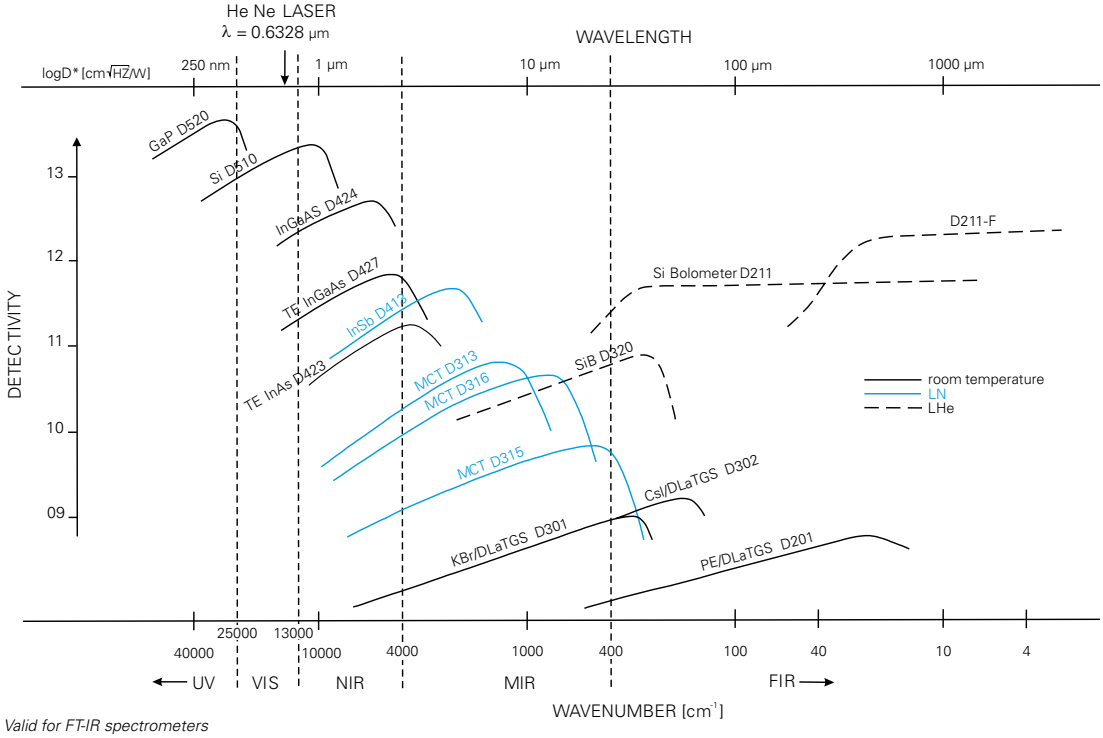
Wavenumber [cm^{-1}]	Wavelength [μm]	Wavelength [nm]	Frequency [GHz]	Electron Volt [eV]
1 000.0	10.00	10 000	29 979	.12 398
1 100.0	9.09	9 091	32 977	.13 638
1 200.0	8.33	8 333	35 975	.14 878
1 300.0	7.69	7 692	38 973	.16 118
1 400.0	7.14	7 143	41 971	.17 358
1 500.0	6.67	6 667	44 968	.18 598
1 600.0	6.25	6 250	47 966	.19 837
1 700.0	5.88	5 882	50 964	.21 077
1 800.0	5.56	5 556	53 962	.22 317
1 900.0	5.26	5 263	56 960	.23 557
2 000.0	5.00	5 000	59 958	.24 797
2 200.0	4.55	4 545	65 954	.27 276
2 400.0	4.17	4 167	71 950	.29 756
2 600.0	3.85	3 846	77 945	.32 236
2 800.0	3.57	3 571	83 941	.34 716
3 000.0	3.33	3 333	89 937	.37 195
3 200.0	3.13	3 125	95 933	.39 675
3 400.0	2.94	2 941	101 929	.42 155
3 600.0	2.78	2 778	107 924	.44 634
3 800.0	2.63	2 632	113 920	.47 114
4 000.0	2.50	2 500	119 916	.49 594
5 000.0	2.00	2 000	149 895	.61 992
6 000.0	1.67	1 667	179 874	.74 390
7 000.0	1.43	1 429	209 853	.86 789
8 000.0	1.25	1 250	239 832	.99 187
9 000.0	1.11	1 111	269 811	1.11 586
10 000.0	1.00	1 000	299 790	1.23 984
11 000.0	.91	909	329 769	1.36 382
12 000.0	.83	833	359 748	1.48 781
13 000.0	.77	769	389 727	1.61 179
14 000.0	.71	714	419 706	1.73 578
15 000.0	.67	667	449 685	1.85 976
16 000.0	.62	625	479 664	1.98 374
17 000.0	.59	588	509 643	2.10 773
18 000.0	.56	556	539 622	2.23 171
19 000.0	.53	526	569 601	2.35 570
20 000.0	.50	500	599 580	2.47 968
22 000.0	.45	455	659 538	2.72 765
24 000.0	.42	417	719 496	2.97 562
26 000.0	.38	385	779 454	3.22 358
28 000.0	.36	357	839 412	3.47 155
30 000.0	.33	333	899 370	3.71 952
32 000.0	.31	312	959 328	3.96 749
34 000.0	.29	294	1 019 286	4.21 546
36 000.0	.28	278	1 079 244	4.46 342
38 000.0	.26	263	1 139 202	4.71 139
40 000.0	.25	250	1 199 160	4.95 936
50 000.0	.20	200	1 498 950	6.19 921

IR Spectroscopy Tables

Sources



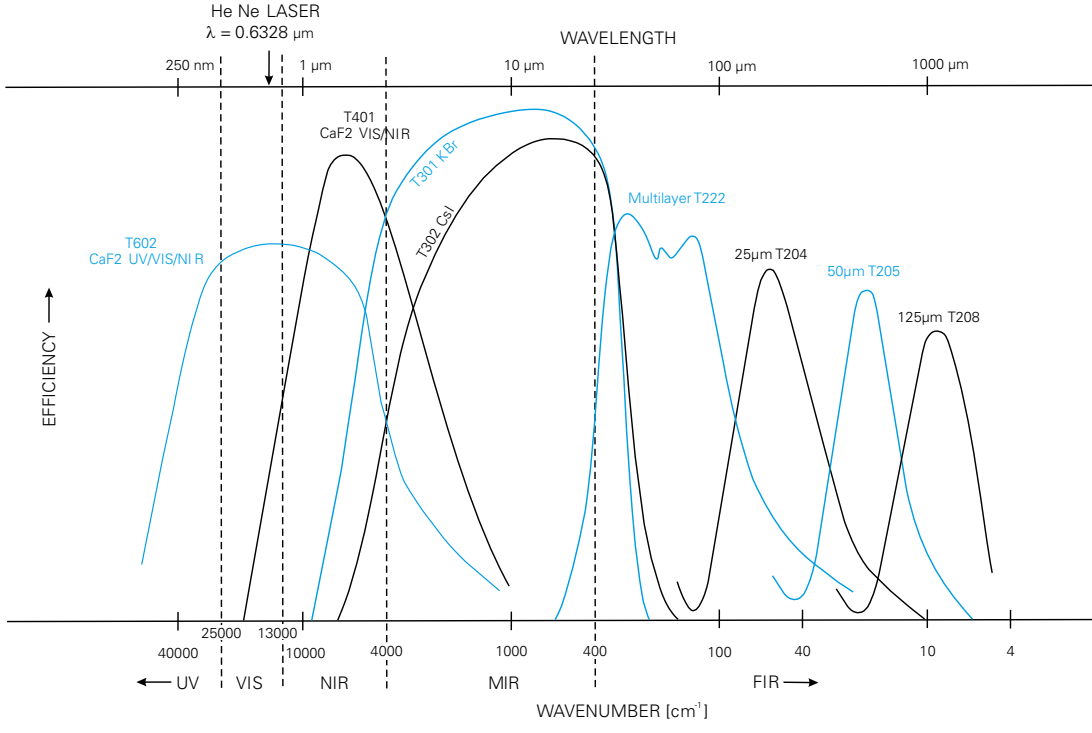
Detectors



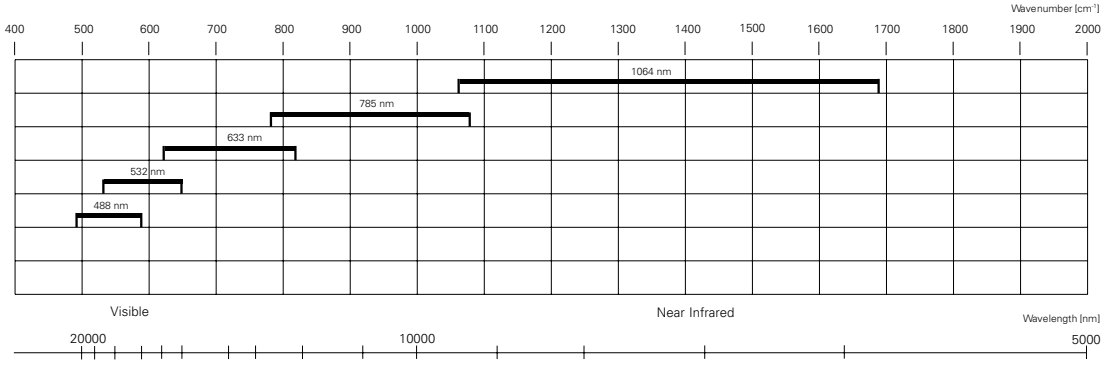
Valid for FT-IR spectrometers

IR Spectroscopy and Raman Tables

Beamsplitters



Stokes Shifts (0-3500 cm^{-1}) of Various Laser Sources



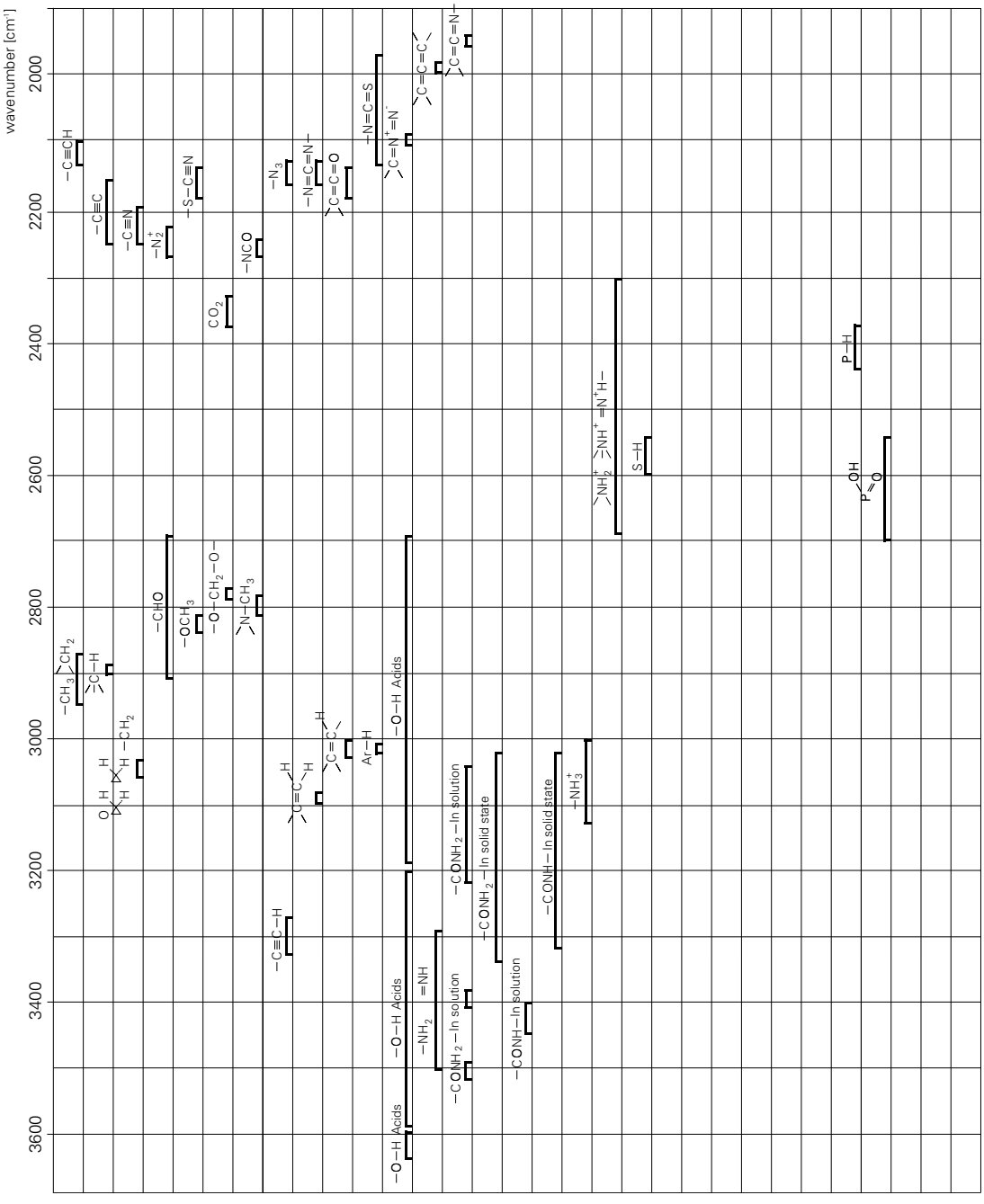
Selected Force Constants and Bond Orders of Organic and Inorganic Compounds (according to Siebert)

Bond A-B	Force Const. f (N cm^{-1})	Bond Order	Compound	Bond A-B	Force Const. f (N cm^{-1})	Bond Order	Compound
H-H	5.14	0.77	H_2	**C-S**	3.3	1.0	$S(CH_3)_2$
Li-Li	1.24	1.2	Li_2	**C-Cl**	3.12	0.93	CCl_4
B-B	3.58	1.2	B_2	**C-Ni**	2.91	1.2	Ni_4CO
C-C	16.5	3.2	HCCH	**C-Ni**	1.43	0.68	NiCO
N-N	22.42	3.2	N_2	**C-Se**	5.94	1.8	CSe_2
O-O	11.41	1.4	O_2	**C-Br**	2.42	0.86	CBr_4
F-F	4.45	0.58	F_2	**C-Rh**	2.4	1.2	$(Rh(CN)_6)^{3-}$
Na-Na	0.17	0.24	Na_2	**C-Ag**	2.0	0.99	$(Ag(CN)_2)^-$
Si-Si	4.65	2.0	Si_2	**C-I**	1.69	0.79	CI_4
Si-Si	~1.7	~0.9	Si_2H_6	**N-H**	7.05	1.1	NH_3
P-P	5.56	2.1	P_2	**N-B**	7.2	1.6	BN_2^{3-}
P-P	2.07	0.95	P_4	**N-C**	18.07	3.0	HCN
S-S	4.96	1.7	S_2	**N-N**	22.42	3.2	N_2
S-S	2.5	0.99	S_8	**N-N**	16.01	2.4	N-NNH
Cl-Cl	3.24	1.1	Cl_2	**N-N**	13.15	2.0	N-N-N$^-$
Ni-Ni	0.11	0.2	Ni solid	**N-O**	25.07	3.1	N-O$^+$
As-As	3.91	1.8	As_2	**N-O**	17.17	2.3	NO^+_2
Se-Se	3.61	1.6	$^{80}Se_2$	**N-O**	15.49	2.1	NO
Br-Br	2.36	1.1	Br_2	**N-O**	15.18	2.0	ONCl
Rb-Rb	0.08	0.2	Rb_2	**N-O**	11.78	1.7	NNO
Cd-Cd	1.11	1.0	Cd_2^{2+}	**N-F**	4.16	0.66	NF_3
Sb-Sb	2.61	1.9	Sb_2	**N-Si**	3.8	1.1	$((CH_3)_3Si)_2NH$
Te-Te	2.37	1.7	Te_2	**N-S**	12.54	2.5	NSF_3
I-I	1.70	1.2	I_2	**N-S**	8.3	1.9	HNSO
Hg-Hg	1.69	1.5	Hg_2^{2+}	**N-S**	3.1	0.87	H_3N-SO_3
Pb-Pb	4.02	3	Pb_2	**O-Li**	1.58	0.66	LiO
Bi-Bi	1.84	1.6	Bi_2	**O-Be**	7.51	1.8	BeO
H-B	2.75	0.68	BH_3	**O-B**	13.66	2.5	BO
H-C	5.50	1.0	CH_4	**O-B**	6.35	1.3	BO_3^{3-}
H-N	7.05	1.1	NH_3	**O-O**	16.59	2.0	O^+_2
H-O	8.45	1.1	H_2O	**O-O**	11.41	1.4	O_2
H-O	7.40	1.0	HO^-	**O-O**	6.18	0.89	O^-_2
H-F	8.85	1.1	HF	**O-O**	5.70	0.83	O_3
H-Al	1.76	0.60	AlH^-_4	**O-Na**	~3.2	~1.1	Na-OH
H-Si	2.98	0.84	SiH_4	**O-Mg**	3.5	1.1	MgO
H-P	3.11	0.82	PH_3	**O-Al**	5.66	1.5	AlO
H-S	4.29	1.0	H_2S	**O-Al**	3.8	1.1	$Al(OH)^-_4$
H-Cl	4.81	1.0	HCl	**O-Si**	9.25	2.1	SiO
H-Ge	2.81	0.82	GeH_4	**O-Si**	4.75	1.2	SiO^{-4}_4
H-As	2.85	0.81	AsH_3	**O-P**	9.41	2.0	PO
H-Se	3.51	0.93	H_2Se	**O-P**	6.16	1.4	PO^{3-}_4
H-Br	3.84	0.98	HBr	**O-S**	10.01	2.0	SO_2
H-Sn	2.03	0.76	SnH_4	**O-Cl**	4.26	1.0	ClO^-_2
H-Sb	2.09	0.77	SbH_3	**O-Cl**	3.30	0.82	ClO^-
H-I	2.92	0.97	HI	**O-Ca**	2.85	1.2	CaO
C-H	5.50	1.0	CH_4	**O-Ti**	7.19	2.4	TiO
C-B	3.82	1.1	$B(CH_3)_3$	**O-V**	7.36	2.3	VO
C-C	16.5	3.2	HCCH	**O-Cr**	5.82	1.9	CrO
C-C	9.15	1.9	H_2CCH_2	**O-Mn**	5.16	1.6	MnO
C-C	7.6	1.7	C_6H_6	**O-Fe**	5.67	1.7	FeO
C-C	4.4	1.1	H_3CCH_3	**O-Cu**	2.97	0.93	CuO
C-N	18.07	3.0	HCN	**O-Ge**	7.53	1.8	^{74}GeO
C-N	11.84	2.1	CN_2^{2-}	**O-Se**	6.45	1.5	SeO
C-N	6.54	1.3	$NNCH_2$	**O-Mo**	3.05	1.2	Ba_2CaMoO_6 (solid)
C-O	18.56	2.8	CO	**O-Ru**	6.70	2.2	RuO_4
C-O	15.61	2.4	CO_2	**O-Ag**	2.00	0.79	AgO
C-O	12.76	2.0	OCH_2	**O-Sn**	5.53	1.7	SnO
C-O	7.86	1.3	CO_3^{2-}	**O-Te**	5.31	1.6	TeO
C-O	5.1	0.96	$O(CH_3)_2$	**O-Ba**	3.79	1.8	BaO
C-F	6.98	1.1	CF_4	**O-Ce**	6.33	2.6	CeO
C-P	8.95	2.4	HCP	**O-Pr**	5.68	2.4	PrO
C-S	7.67	2.0	CS_2	**O-Nd**	3.5	1.6	$NdAc_3 \cdot H_2O$ (polymer)

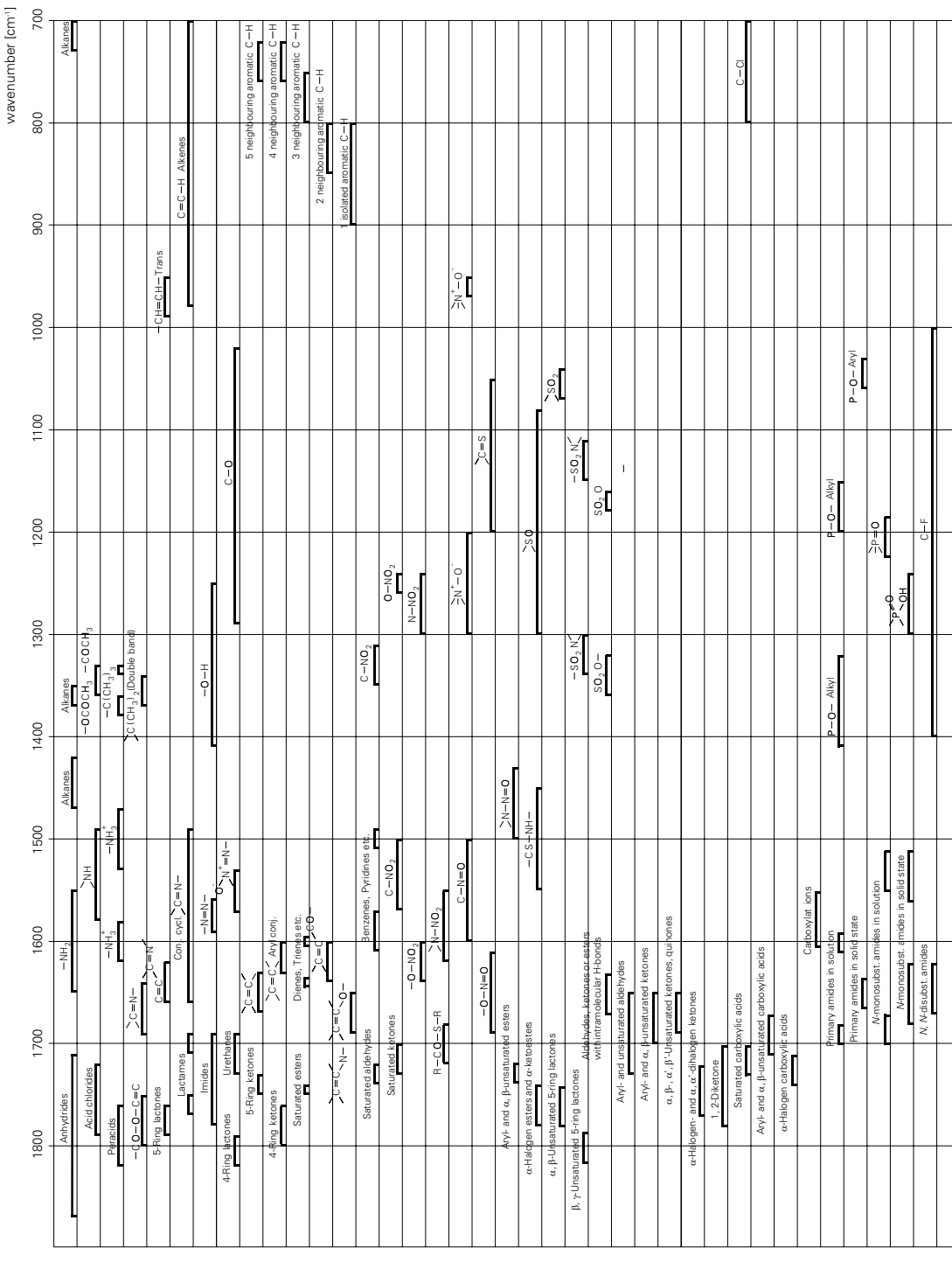
IR Window Materials

Material	Transmission Range [cm^{-1}] ([micrometers])	Refractive Index n at 2000 cm^{-1}	Reflectance loss per surface	Hardness (Knoop)	Chemical Properties
Infrasil SiO_2	57,000-2,800 (0.175-3.6)	1.46	~ 3.3%	461	Insoluble in water; soluble in HF.
UV Sapphire AL_2O_3	66,000-2,000 (0.15-5.0)	1.75	~ 7.3%	1370	Very slightly soluble in acids and bases.
Silicon Si	10,000-100 (1.0-100)	3.42	~ 30%	1150	Insoluble in most acids and bases; soluble in HF and HNO_3.
Calcium Fluoride CaF_2	66,000-1,200 (0.15-8.0)	1.40	~ 2.8%	158	Insoluble in water; resists most acids and bases; soluble in NH_4 salts.
Barium Fluoride BaF_2	50,000-900 (0.2-11)	1.45	~ 3.3%	82	Low water solubility; soluble in acid and NH_4Cl.
Zinc Sulfide, Cleartran ZnS	22,000-750 (0.45-13.0)	2.25	~ 15%	355	Soluble in acid; insoluble in water.
Germanium Ge	5,000-600 (2.0-17)	4.01	~ 36%	550	Insoluble in water; soluble in hot H_2SO_4 and aqua regia.
Sodium Chloride NaCl	28,000-700 (0.35-15)	1.52	~ 4.5%	15	Hygroscopic; slightly soluble in alcohol and NH_3.
AMTIR GeAsSe Glass	11,000-900 (0.9-11)	2.50	~ 18%	170	Insoluble in water. Soluble in bases.
Zinc Selenide ZnSe	20,000-500 (0.5-20)	2.43	~ 17%	150	Soluble in strong acids; dissolves in HNO_3.
Silver Chloride AgCl	23,000-400 (0.42-25)	2.00	~ 11%	10	Insoluble in water; soluble in NH_4OH.
Potassium Bromide KBr	33,000-400 (0.3-25)	1.54	~ 4.5%	7	Soluble in water, alcohol, and glycerine; hygroscopic.
Cesium Iodide CsI	33,000-150 (0.3-70)	1.74	~ 7.3%	20	Soluble in water and alcohol; hygroscopic.
KRS-5 TlBr/I	16,000-200 (0.6-60)	2.38	~ 17%	40	Soluble in warm water; soluble in bases; insoluble in acids.
Polyethylene PE (high density)	600-10 (16-1,000)	1.52	~ 4.5%	5	Resistant to most solvents.
Diamond C	45,000-10 (0.22-1,000)	2.40	~ 17%	7000	Insoluble in water, acids, and bases.
TPX(TM) Methylpentene Resin	350-10 (28-1,000)	1.43	~ 3.3%		Similar to PE but transparent and more rigid.

Infrared Tables



Infrared Tables



MS: Exact Masses of the Isotopes

Atomic Masses and Representative Abundances of the Isotopes (NIST)

The masses and abundances of the isotopes we use for generating molecular formulas, simulating patterns and SNAP peak finding basically are taken from the National Institute of Standards and Technology (NIST).

Z = Atomic number, M = mass number; Ratios are calculated with most abundant isotope = 1.

Z	E	M	Exact Mass	Abund.	Valency
1	H	1	1.0078250321	0.999885	1
	D	2	2.0141017778	0.000115	
	T	3	3.0160492777		
2	He	3	3.0160293191	1.34e-6	0
		4	4.0026032541	0.99999866	
3	Li	6	6.015122795	0.0759	1
		7	7.01600455	0.9241	
4	Be	9	9.0121822	1	2
5	B	10	10.0129370	0.199	3
		11	11.0093054	0.801	
6	C	12	12 (by definition)	0.9893	4
		13	13.003354837	0.0107	
		14	14.003241989		
7	N	14	14.003074004	0.99636	3
		15	15.000108982	0.00364	
8	O	16	15.994914619	0.99757	2
		17	16.99913170	0.00038	
		18	17.9991610	0.00205	
9	F	19	18.99840322	1	1
10	Ne	20	19.992440175	0.9048	0
		21	20.99384668	0.0027	
		22	21.991385114	0.0925	
11	Na	23	22.98976928	1	1
12	Mg	24	23.985041700	0.7899	2
		25	24.98583692	0.1000	
		26	25.982592929	0.1101	
13	Al	27	26.98153863	1	3
14	Si	28	27.976926532	0.92223	4
		29	28.976494700	0.04685	
		30	29.97377017	0.03092	
15	P	31	30.97376163	1	3
		32	31.97390727		
16	S	32	31.97207100	0.9499	2
		33	32.97145876	0.0075	
		34	33.96786690	0.0425	
		36	35.96708076	0.0001	
17	Cl	35	34.96885268	0.7576	1
		37	36.96590259	0.2424	
18	Ar	36	35.967545106	0.003365	0
		38	37.9627324	0.000632	
		40	39.962383122	0.996003	
19	K	39	38.96370668	0.932581	1
		40	39.96399848	0.000117	
		41	40.96182576	0.067302	
20	Ca	40	39.96259098	0.96941	2
		42	41.95861801	0.00647	
		43	42.9587666	0.00135	
		44	43.9554818	0.02086	
		46	45.9536926	0.00004	
		48	47.952534	0.00187	
21	Sc	45	44.9559119	1	3
22	Ti	46	45.9526316	0.0825	4
		47	46.9517631	0.0744	
		48	47.9479463	0.7372	
		49	48.9478700	0.0541	
		50	49.9447912	0.0518	
23	V	50	49.9471585	0.00250	5
		51	50.9439595	0.99750	
24	Cr	50	49.9460442	0.04345	3
		52	51.9405075	0.83789	
		53	52.9406494	0.09501	
		54	53.9388804	0.02365	
25	Mn	55	54.9380451	1	2
26	Fe	54	53.9396105	0.05845	2
		56	55.9349375	0.91754	
		57	56.9353940	0.02119	
		58	57.9332756	0.00282	
27	Co	59	58.9331950	1	2
28	Ni	58	57.9353429	0.680769	2
		60	59.9307864	0.262231	
		61	60.9310560	0.011399	
		62	61.9283451	0.036345	
		64	63.9279660	0.009256	

MS: Exact Masses of the Isotopes

BRUKER

Atomic Masses and Representative Abundances of the Isotopes (NIST)

The masses and abundances of the isotopes we use for generating molecular formulas, simulating patterns and SNAP peak finding basically are taken from the National Institute of Standards and Technology (NIST).

Z = Atomic number, M = mass number; Ratios are calculated with most abundant isotope = 1.

Z	E	M	Exact Mass	Abund.	Valency
29	Cu	63	62.9295975	0.6915	1
		65	64.9277895	0.3085	
30	Zn	64	63.9291422	0.48268	2
		66	65.9260334	0.27975	
		67	66.9271273	0.04102	
		68	67.9248442	0.19024	
		70	69.9253193	0.00631	
31	Ga	69	68.9255736	0.60108	3
		71	70.9247013	0.39892	
32	Ge	70	69.9242474	0.2038	4
		72	71.9220758	0.2731	
		73	72.9234589	0.0776	
		74	73.9211778	0.3672	
		76	75.9214026	0.0783	
33	As	75	74.9215965	1	3
34	Se	74	73.9224764	0.0089	2
		76	75.9192136	0.0937	
		77	76.9199140	0.0763	
		78	77.9173091	0.2377	
		80	79.9165213	0.4961	
		82	81.9166994	0.0873	
35	Br	79	78.9183371	0.5069	1
		81	80.9162906	0.4931	
36	Kr	78	77.9203648	0.00355	0
		80	79.9163790	0.02286	
		82	81.9134836	0.11593	
		83	82.914136	0.11500	
		84	83.911507	0.56987	
		86	85.91061073	0.17279	
37	Rb	85	84.911789738	0.7217	1
		87	86.909180527	0.2783	
38	Sr	84	83.913425	0.0056	2
		86	85.9092602	0.0986	
		87	86.9088771	0.0700	
		88	87.9056121	0.8258	
39	Y	89	88.9058483	1	3
40	Zr	90	89.9047044	0.5145	4
		91	90.9056458	0.1122	
		92	91.9050408	0.1715	
		94	93.9063152	0.1738	
		96	95.9082734	0.0280	
41	Nb	93	92.9063781	1	5
42	Mo	92	91.906811	0.1477	6
		94	93.9050883	0.0923	
		95	94.9058421	0.1590	
		96	95.9046795	0.1668	
		97	96.9060215	0.0956	
		98	97.9054082	0.2419	
		100	99.907477	0.0967	
43	Tc	97	96.906365		4
		98	97.907216		
		99	98.9062547		
44	Ru	96	95.907598	0.0554	3
		98	97.905287	0.0187	
		99	98.9059393	0.1276	
		100	99.9042195	0.1260	
		101	100.9055821	0.1706	
		102	101.9043493	0.3155	
		104	103.905433	0.1862	
45	Rh	103	102.905504	1	3
46	Pd	102	101.905609	0.0102	2
		104	103.904036	0.1114	
		105	104.905085	0.2233	
		106	105.903486	0.2733	
		108	107.903892	0.2646	
		110	109.905153	0.1172	
47	Ag	107	106.905097	0.51839	1
		109	108.904752	0.48161	
48	Cd	106	105.906459	0.0125	2
		108	107.904184	0.0089	
		110	109.903021	0.1249	
		111	110.904178	0.1280	
		112	111.9027578	0.2413	
		113	112.9044017	0.1222	
		114	113.9033585	0.2873	
		116	115.904756	0.0749	

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BRUKER

Atomic Masses and Representative Abundances of the Isotopes (NIST)

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Z	E	M	Exact Mass	Abund.	Valency
49	In	**113**	112.904058	0.0429	3
		115	114.903878	0.9571	
50	Sn	**112**	111.904818	0.0097	4
		114	113.902779	0.0066	
		115	114.903342	0.0034	
		116	115.901741	0.1454	
		117	116.902952	0.0768	
		118	117.901603	0.2422	
		119	118.903308	0.0859	
		120	119.9021947	0.3258	
		122	121.9034390	0.0463	
		124	123.9052739	0.0579	
51	Sb	**121**	120.9038157	0.5721	5
		123	122.9042140	0.4279	
52	Te	**120**	119.904020	0.0009	2
		122	121.9030439	0.0255	
		123	122.9042700	0.0089	
		124	123.9028179	0.0474	
		125	124.9044307	0.0707	
		126	125.9033117	0.1884	
		128	127.9044631	0.3174	
		130	129.9062244	0.3408	
53	I	**127**	126.904473	1	1
54	Xe	**124**	123.9058930	0.000952	0
		126	125.904274	0.000890	
		128	127.9035313	0.019102	
		129	128.9047794	0.264006	
		130	129.9035080	0.040710	
		131	130.9050824	0.212324	
		132	131.9041535	0.269086	
		134	133.9053945	0.104357	
		136	135.907219	0.088573	
55	Cs	**133**	132.905451933	1	1
56	Ba	**130**	129.9063208	0.00106	2
		132	131.9050613	0.00101	
		134	133.9045084	0.02417	
		135	134.9056886	0.06592	
		136	135.9045759	0.07854	
		137	136.9058274	0.11232	
		138	137.9052472	0.71698	
57	La	**138**	137.907112	0.00090	3
		139	138.9063533	0.99910	
58	Ce	**136**	135.907172	0.00185	4
		138	137.905991	0.00251	
		140	139.9054387	0.88450	
		142	141.909244	0.11114	
59	Pr	**141**	140.9076528	1	3
60	Nd	**142**	141.9077233	0.272	3
		143	142.9098143	0.122	
		144	143.9100873	0.238	
		145	144.9125736	0.083	
		146	145.9131169	0.172	
		148	147.916893	0.057	
		150	149.920891	0.056	
61	Pm	**145**	144.912749		
		147	146.9151385		
62	Sm	**144**	143.911999	0.0307	2
		147	146.9148979	0.1499	
		148	147.9148227	0.1124	
		149	148.9171847	0.1382	
		150	149.9172755	0.0738	
		152	151.9197324	0.2675	
		154	153.9222093	0.2275	
63	Eu	**151**	150.9198502	0.4781	2
		153	152.9212303	0.5219	
64	Gd	**152**	151.9197910	0.0020	3
		154	153.9208656	0.0218	
		155	154.9226220	0.1480	
		156	155.9221227	0.2047	
		157	156.923601	0.1565	
		158	157.9241039	0.2484	
		160	159.9270541	0.2186	
65	Tb	**159**	158.9253468	1	3
66	Dy	**156**	155.924283	0.00056	3
		158	157.924409	0.00095	
		160	159.9251975	0.02329	
		161	160.9269334	0.18889	
		162	161.9267984	0.25475	
		163	162.9287312	0.24896	
		164	163.9291748	0.28260	

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Z	E	M	Exact Mass	Abund.	Valency
67	Ho	**165**	164.9303221	1	3
68	Er	**162**	161.928778	0.00139	3
		164	163.929200	0.01601	
		166	165.9302931	0.33503	
		167	166.9320482	0.22869	
		168	167.9323702	0.26978	
		170	169.9354643	0.14910	
69	Tm	**169**	168.9342133	1	3
70	Yb	**168**	167.933897	0.0013	2
		170	169.9347618	0.0304	
		171	170.9363258	0.1428	
		172	171.9363815	0.2183	
		173	172.9382108	0.1613	
		174	173.9388621	0.3183	
		176	175.9425717	0.1276	
71	Lu	**175**	174.9407718	0.9741	3
		176	175.9426863	0.0259	
72	Hf	**174**	173.940046	0.0016	4
		176	175.9414086	0.0526	
		177	176.9432207	0.1860	
		178	177.9436988	0.2728	
		179	178.9458161	0.1362	
		180	179.9465500	0.3508	
73	Ta	**180**	179.9474648	0.00012	5
		181	180.9479958	0.99988	
74	W	**180**	179.946704	0.0012	6
		182	181.9482042	0.2650	
		183	182.9502230	0.1431	
		184	183.9509312	0.3064	
		186	185.9543641	0.2843	
75	Re	**185**	184.9529550	0.3740	4
		187	186.9557531	0.6260	
76	Os	**184**	183.9524891	0.0002	3
		186	185.9538382	0.0159	
		187	186.9557505	0.0196	
		188	187.9558382	0.1324	
		189	188.9581475	0.1615	
		190	189.9584470	0.2626	
		192	191.9614807	0.4078	
77	Ir	**191**	190.9605940	0.373	3
		193	192.9629264	0.627	
78	Pt	**190**	189.959932	0.00014	2
		192	191.9610380	0.00782	
		194	193.9626803	0.32967	
		195	194.9647911	0.33832	
		196	195.9649515	0.25242	
		198	197.967893	0.07163	
79	Au	**197**	196.9665687	1	1
80	Hg	**196**	195.965833	0.0015	2
		198	197.9667690	0.0997	
		199	198.9682799	0.1687	
		200	199.9683260	0.2310	
		201	200.9703023	0.1318	
		202	201.9706430	0.2986	
		204	203.9734939	0.0687	
81	Tl	**203**	202.9723442	0.2952	3
		205	204.9744275	0.7048	
82	Pb	**204**	203.9730436	0.014	4
		206	205.9744653	0.241	
		207	206.9758969	0.221	
		208	207.9766521	0.524	
83	Bi	**209**	208.9803987	1	5
90	Th	**232**	232.0380553	1	4
91	Pa	**231**	231.0358840	1	4
92	U	**234**	234.0409521	5.4e-05	3
		235	235.0439299	0.007204	
		238	238.0507882	0.992742	

References:

Coursey, J.S., Schwab, D.J., and Dragoset, R.A. (2003), Atomic Weights and Isotopic Compositions (version 3.0). [Online] Available: http://www.nist.gov/physlab/data/comp.cfm [2010, July 15]. National Institute of Standards and Technology, Gaithersburg, MD.

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The following modifications/additions were made to the NIST Atomic Weights and Isotopic Compositions (version 3.0) table:

- Additional elements Ct, Nt and Ot were defined which have an abundance of 95 % of 13C, 15N and 18O and 5 % of 12C, 14N and 16O. These elements were added to calculate isotopically marked substances. Within the software the complete list of atoms and isotopes is available.
- Typical valencies of the atoms are listed additionally. For quickly inspecting the valencies used, please refer to the Table of Valencies.

Solid-Phase Peptide Synthesis

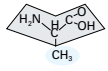
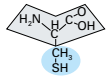
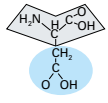
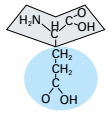
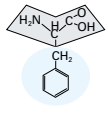
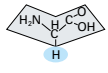
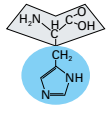
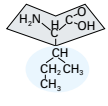
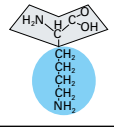
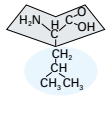
Mass Shift of Modifications, Protection Groups and Artifacts

m/z shift [Da]	Modification	Abbreviation	Sum formula change	Valid residues	Origin
-186,07931	Trp->Null		$-C_{11}H_{10}N_2O$	W	Deletion
-163,06333	Tyr->Null		$-C_9H_9NO_2$	Y	Deletion
-156,10111	Arg->Null		$-C_6H_{12}N_4O$	R	Deletion
-147,06841	Phe->Null		$-C_9H_9NO$	F	Deletion
-137,05891	His->Null		$-C_6H_7N_3O$	H	Deletion
-131,04049	Met->Null		$-C_5H_9NOS$	M	Deletion
-129,04259	Glu->Null		$-C_5H_7NO_3$	E	Deletion
-128,09496	Lys->Null		$-C_6H_{12}N_2O$	K	Deletion
-128,05858	Gln->Null		$-C_5H_8N_2O_2$	Q	Deletion
-115,02694	Asp->Null		$-C_4H_5NO_3$	D	Deletion
-114,04293	Asn->Null		$-C_4H_6N_2O_2$	N	Deletion
-113,08406	Ile->Null		$-C_6H_{11}NO$	I	Deletion
-113,08406	Leu->Null		$-C_6H_{11}NO$	L	Deletion
-101,04768	Thr->Null		$-C_4H_7NO_2$	T	Deletion
-99,06841	Val->Null		$-C_5H_9NO$	V	Deletion
-97,05276	Pro->Null		$-C_5H_7NO$	P	Deletion
-87,03203	Ser->Null		$-C_3H_5NO_2$	S	Deletion
-71,03711	Ala->Null		$-C_3H_5NO$	A	Deletion
-57,02146	Gly->Null		$-C_2H_3NO$	G	Deletion
-16,01872	Pyro-glutamination (N-term)		$-NH_2$	Q	N-terminal
0,98402	Deamidation		$-NH_2+OH$	NQ	Artefact
14,01565	Methylation		$+CH_2$	DEKR	Chemical Modification
14,01565	Methylation	Me	$-H+CH_3$	Y	Fmoc
15,99492	Oxidation	Ox	+O	MW	Artefact
16,01872	Amidation (C-term)		$-O+NH_2O$	all Amino acids	C-terminal
27,99492	Formylation	For	-H+CHO	W	Boc
28,03130	Dimethylation		$+C_2H_4$	KR	Chemical Modification
28,03130	Ethylation	Et	$-H+C_2H_5$	Y	Boc
29,00274	Formyl (N-term)		+CHO	M	N-terminal
31,98983	Double Oxidation Tryptophane		$+O_2$	W	Artefact
42,01057	Acetylation	Ac	$-H+C_2H_3O$	K	Fmoc
42,04695	Trimethylation		$+C_3H_6$	KR	Chemical Modification
44,98508	Nitration	NO2	$-H+NO_2$	Y	Chemical Modification
44,98508	Nitration	NO2	$-H+NO_2$	R	Boc
47,94445	Selenocystein		-S+Se	C	Chemical Modification
56,06260	Diethylation		$+C_4H_8$	K	Chemical Modification
56,06260	tert.-Butyl	tBu	$-H+C_4H_9$	CSTY	Fmoc
56,06260	tert.-Butyl	tBu	$-H+C_4H_9$	STY	Boc
57,02146	Gly->GG		$+C_2H_3NO$	G	Double coupling
68,06260	Piperidine	Pip	$+C_5H_8$	DE	Artefact
71,03711	Propionamidation		$+C_3H_5NO$	C	Cys-State
71,03711	Ala->AA		$+C_3H_5NO$	A	Double coupling
71,03711	Acetamidomethyl	Acm	$-H+C_3H_6NO$	C	Fmoc/Boc
72,05752	tert.-Butoxy	OtBu	$-H+C_4H_9O$	DE	Fmoc/Boc
79,96633	Phosphorylation		$-H+PO_3H_2$	STY	Chemical Modification
86,07317	tert.-Butoxymethyl	Bum	$-H+C_5H_{11}O$	H	Fmoc
87,03203	Ser->SS		$+C_3H_5NO_2$	S	Double coupling
88,03467	tert.-Butylthio	tButhio	$-H+C_4H_9S$	C	Fmoc
90,04695	Benzyl	Bzl	$-H+C_7H_7$	CST	Fmoc
90,04695	Benzyl	Bzl	$-H+C_7H_7$	CSTY	Boc
95,98230	Trifluoroacetylation	Tfa	$-H+C_2F_3O$	K	Fmoc/Boc
97,05276	Pro->PP		$+C_5H_7NO$	P	Double coupling
99,06841	Val->VV		$+C_5H_9NO$	V	Double coupling
100,05243	tert.-Butoxycarbonyl	Boc	$-H+C_5H_9O_2$	all Amino acids	Boc

Mass Shift of Modifications, Protection Groups and Artifacts

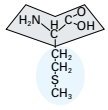
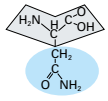
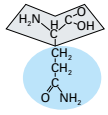
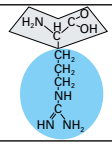
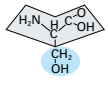
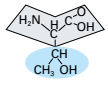
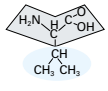
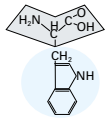
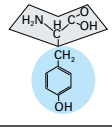
m/z shift [Da]	Modification	Abbreviation	Sum formula change	Valid residues	Origin
101,04768	Thr->TT		$+C_4H_7NO_2$	T	Double coupling
103,00918	Cys->CC		$+C_3H_5NOS$	C	Double coupling
104,06260	4-Methylbenzyl	MeBzl	$-H+C_8H_9$	C	Boc
106,04187	Benzyloxy	BzlO	$-H+C_7H_7O$	DE	Fmoc/Boc
113,08406	Ile->II		$+C_6H_{11}NO$	I	Double coupling
113,08406	Leu->LL		$+C_6H_{11}NO$	L	Double coupling
114,04293	Asn->NN		$+C_4H_6N_2O_2$	N	Double coupling
115,02694	Asp->DD		$+C_4H_5NO_3$	D	Double coupling
118,07825	2-Phenylisopropyl	O-2-PhiPr	$-H+C_9H_{11}$	DE	Fmoc
120,05752	4-Methoxybenzyl	MeOBzl	$-H+C_8H_9O$	C	Fmoc/Boc
120,05752	Benzyloxymethyl	Bom	$-H+C_8H_9O$	H	Boc
128,05858	Gln->QQ		$+C_5H_8N_2O_2$	Q	Double coupling
128,09496	Lys->KK		$+C_6H_{12}N_2O$	K	Double coupling
129,04259	Glu->EE		$+C_5H_7NO_3$	E	Double coupling
131,04049	Met->MM		$+C_5H_9NOS$	M	Double coupling
134,03678	Benzyloxycarbonyl	Z	$-H+C_8H_7O_2$	K	Fmoc/Boc
137,05891	His->HH		$+C_6H_7N_3O$	H	Double coupling
147,06841	Phe->FF		$+C_9H_9NO$	F	Double coupling
148,08882	Adamantyloxy	O-1-Ada	$-H+C_{10}H_{13}O$	D	Fmoc/Boc
148,08882	Adamantyloxy	O-2-Ada	$-H+C_{10}H_{13}O$	D	Boc
154,00885	Tosyl	Tos	$-H+C_7H_7O_2S$	HR	Fmoc/Boc
156,10111	Arg->RR		$+C_6H_{12}N_4O$	R	Double coupling
157,96901	2,6-Dichlorobenzyl	di-Cl-Bzl	$-H+C_7H_5Cl_2$	Y	Fmoc/Boc
163,06333	Tyr->YY		$+C_9H_9NO_2$	Y	Double coupling
164,08373	1-(4,4-Dimethyl-2,6-dioxo-cyclohexylidene)-ethyl	Dde	$-H+C_{10}H_{13}O_2$	K	Fmoc
166,00146	2,4-Dinitrophenyl	Dnp	$-H+C_6H_3N_2O_4$	H	Boc
167,99781	2-Chlorobenzyloxycarbonyl	2-Cl-Z	$-H+C_8H_6ClO_2$	K	Fmoc/Boc
180,05752	Xanthyl	Xan	$-H+C_{13}H_9O$	NQ	Boc
180,07864	2,4,6-Trimethoxybenzyl	Tmob	$-H+C_{10}H_{13}O_3$	N	Fmoc
182,04015	Mesitylene-2-sulfonyl	Mts	$-H+C_9H_{11}O_2S$	R	Fmoc
182,04015	Mesitylene-2-sulfonyl	Mts	$-H+C_9H_{11}O_2S$	RW	Boc
186,07931	Trp->WW		$+C_{11}H_{10}N_2O$	W	Double coupling
206,13068	1-(4,4-Dimethyl-2,6-dioxo-cyclohexylidene)-3-methylbutyl	ivDde	$-H+C_{13}H_{19}O_2$	K	Fmoc
211,94729	2-Bromobenzyloxycarbonyl	2-Br-Z	$-H+C_8H_6BrO_2$	Y	Boc
212,05072	4-Methoxy-2,3,6-trimethyl-benzenesulfonyl	Mtr	$-H+C_{10}H_{13}O_3S$	R	Fmoc/Boc
222,06808	Fluorenylmethoxycarbonyl	Fmoc	$-H+C_{15}H_{11}O_2$	all Amino acids	Fmoc
226,07760	Biotinylation		$+C_{10}H_{14}N_2S_1O_2$	K	Chemical Modification
226,09938	4,4'-Dimethoxybenzhydryl	Mbh	$-H+C_{15}H_{15}O_2$	NQ	Fmoc
242,10955	Trityl	Trt	$-H+C_{19}H_{15}$	CHNQST	Fmoc
242,10955	Trityl	Trt	$-H+C_{19}H_{15}$	CHNQ	Boc
252,08202	2,2,4,6,7-Pentamethyl-dihydrobenzofurane-5-sulfonyl	Pbf	$-H+C_{13}H_{17}O_3S$	R	Fmoc
256,12520	4-Methyltrityl	Mtt	$-H+C_{20}H_{17}$	HK	Fmoc
266,09767	2,2,5,7,8-Pentamethyl-chromane-6-sulfonyl	Pmc	$-H+C_{14}H_{19}O_3S$	R	Fmoc
272,12012	4-Methoxytrityl	Mmt	$-H+C_{20}H_{17}O$	C	Fmoc
276,07058	2-Chlorotrityl	2-Cl-Trt	$-H+C_{19}H_{14}Cl$	Y	Fmoc
327,18344	4{N-[1-(4,4-Dimethyl-2,6-dioxo-cyclohexylidene)-3-methylbutyl]-amino}benzyloxy	ODmab	$-H+C_{20}H_{26}NO_3$	DE	Fmoc
388,08211	Fluorescein		$+C_{22}H_{14}N_1O_6$	C	Chemical Modification
421,07324	Fluoresceinisothiocyanat	FITC	$+C_{21}S_1H_{15}N_3O_5$	CKRS	Chemical Modification
431,26920	Biotinylation		$-H+C_{20}H_{40}N_4O_4S$	K	Chemical Modification
672,29816	CyDye-Cy3		$+C_{37}H_{44}N_4S_1O_6$	C	Chemical Modification

Molecular Weights of Amino Acid Residues

Amino Acid Structure	Name	Symbol	1 Letter Code	Elemental Composition (Residue)	Monoisotopic Mass (Residue)	Averaged Mass (Residue)
	Alanine	Ala	A	C_3H_5NO	71.03712	71.08
	Cysteine	Cys	C	C_3H_5NOS	103.00919	103.15
	Aspartic acid	Asp	D	$C_4H_5NO_3$	115.02695	115.09
	Glutamic acid	Glu	E	$C_5H_7NO_3$	129.0426	129.12
	Phenylanaline	Phe	F	C_9H_9NO	147.06842	147.18
	Glycine	Gly	G	C_2H_3NO	57.02146	57.05
	Histidine	His	H	$C_6H_7N_3O$	137.05891	137.14
	Isoleucine	Ile	I	$C_6H_{11}NO$	113.08407	113.16
	Lysine	Lys	K	$C_6H_{12}N_2O$	128.09497	128.17
	Leucine	Leu	L	$C_6H_{11}NO$	113.08407	113.16

Masses of Terminal Groups

C-Terminal Groups	Composition	Monoisotopic Mass	Averaged Mass
Free Acid	OH	17.00274	17.00735
Amide	NH_2	16.01872	16.02262

Amino Acid Structure	Name	Symbol	1 Letter Code	Elemental Composition (Residue)	Monoisotopic Mass (Residue)	Averaged Mass (Residue)
	Methionine	Met	M	C_5H_9NOS	131.04049	131.20
	Asparagine	Asn	N	$C_4H_6N_2O_2$	114.04293	114.10
	Proline	Pro	P	C_5H_7NO	97.05277	97.12
	Glutamine	Gln	Q	$C_5H_8N_2O_2$	128.05858	128.13
	Arginine	Arg	R	$C_6H_{12}N_4O$	156.10112	156.19
	Serine	Ser	S	$C_3H_5NO_2$	87.03203	87.08
	Threonine	Thr	T	$C_4H_7NO_2$	101.04768	101.11
	Valine	Val	V	C_5H_9NO	99.06842	99.13
	Tryptophan	Trp	W	$C_{11}H_{10}N_2O$	186.07932	186.21
	Tyrosine	Tyr	Y	$C_9H_9NO_2$	163.06333	163.18

N-Terminal Groups	Composition	Monoisotopic Mass	Averaged Mass
Hydrogen	H	1.00783	1.0079
N-Formyl	HCO	29.00274	29.01808
N-Acetyl	CH_3CO	43.01839	43.04447

Amino Acid Calculator Table

Residues Sorted by Molecular Weight

Sums and Differences of 2 Amino Acid Residues Residue Mass Differences

		G	A	S	P	V	T	C	I	L
		57.05203	**71.07902**	**87.07832**	**97.11704**	**99.13299**	**101.10531**	**103.14344**	**113.15998**	**113.15998**
G	**57.05203**	114.10406	14.02699	30.02629	40.06501	42.08097	44.05328	46.09141	56.10795	56.10795
A	**71.07902**	128.13105	**142.15804**	15.99931	26.03803	28.05398	30.02629	32.06442	42.08097	42.08097
S	**87.07832**	144.13035	158.15734	**174.15665**	10.03872	12.05467	14.02699	16.06512	26.08166	26.08166
P	**97.11704**	154.16907	168.19606	184.19537	**194.23409**	2.01595	3.98827	6.02640	16.04294	16.04294
V	**99.13299**	156.18502	170.21201	186.21132	196.25004	**198.26599**	1.97232	4.01045	14.02699	14.02699
T	**101.10531**	158.15734	172.18433	188.18363	198.22235	200.23831	**202.21062**	2.03813	12.05467	12.05467
C	**103.14344**	160.19547	174.22246	190.22176	200.26048	202.27644	204.24875	**206.28688**	10.01654	10.01654
I	**113.15998**	170.21201	184.23900	200.23831	210.27703	212.29298	214.26529	216.30342	**226.31997**	**0.00000**
L	**113.15998**	170.21201	184.23900	200.23831	210.27703	212.29298	214.26529	216.30342	226.31997	**226.31997**
N	114.10406	171.15609	185.18308	201.18238	211.22110	213.23705	215.20937	217.24750	227.26404	227.26404
D	**115.08866**	172.14069	186.16768	202.16699	212.20571	214.22166	216.19398	218.23211	228.24865	228.24865
Q	128.13105	185.18308	199.21006	215.20937	225.24809	227.26404	229.23636	231.27449	241.29103	241.29103
K	**128.17468**	185.22671	199.25370	215.25300	225.29172	227.30768	229.27999	231.31812	241.33466	241.33466
E	**129.11565**	186.16768	200.19467	216.19398	226.23270	228.24865	230.22096	232.25909	242.27564	242.27564
M	**131.19742**	188.24945	202.27644	218.27574	228.31446	230.33041	232.30273	234.34086	244.35740	244.35740
H	**137.14152**	194.19355	208.22054	224.21985	234.25857	236.27452	238.24684	240.28497	250.30151	250.30151
F	**147.17714**	204.22917	218.25616	234.25546	244.29418	246.31014	248.28245	250.32058	260.33712	260.33712
R	156.18813	213.24016	227.26714	243.26645	253.30517	255.32112	257.29344	259.33157	269.34811	269.34811
Y	**163.17645**	220.22848	234.25546	250.25477	260.29349	262.30944	264.28176	266.31989	276.33643	276.33643
W	186.21391	243.26594	257.29293	273.29224	283.33096	285.34691	287.31922	289.35735	299.37390	299.37390

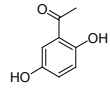
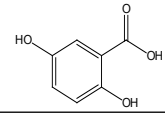
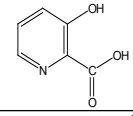
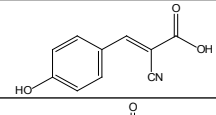
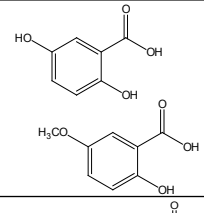
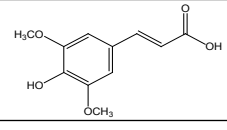
Amino Acid Calculator Table

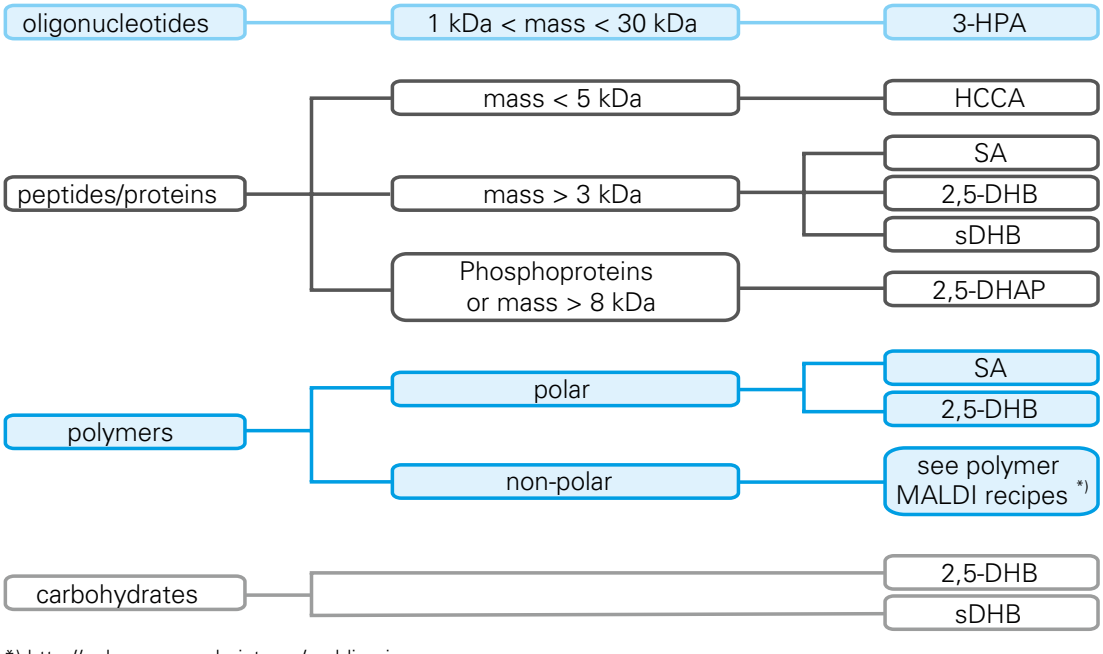
N	D	Q	K	E	M	H	F	R	Y	W
114.10406	**115.08866**	**128.13105**	**128.17468**	**129.11565**	**131.19742**	**137.14152**	**147.17714**	**156.18813**	**163.17645**	**186.21391**
57.05203	58.03664	71.07902	71.12265	72.06362	74.14539	80.08950	90.12511	99.13610	106.12442	129.16188
43.02504	44.00965	57.05203	57.09566	58.03664	60.11840	66.06251	76.09812	85.10911	92.09743	115.13490
27.02574	28.01034	41.05272	41.09636	42.03733	44.11910	50.06320	60.09882	69.10980	76.09812	99.13559
16.98702	17.97162	31.01400	31.05764	31.99861	34.08038	40.02448	50.06010	59.07108	66.05940	89.09687
14.97106	15.95567	28.99805	29.04169	29.98266	32.06442	38.00853	48.04415	57.05513	64.04345	87.08092
12.99875	13.98335	27.02574	27.06937	28.01034	30.09211	36.03621	46.07183	55.08282	62.07113	85.10860
10.96062	11.94522	24.98761	25.03124	25.97221	28.05398	33.99808	44.03370	53.04469	60.03301	83.07047
0.94407	1.92868	14.97106	15.01470	15.95567	18.03744	23.98154	34.01716	43.02814	50.01646	73.05393
0.94407	1.92868	14.97106	15.01470	15.95567	18.03744	23.98154	34.01716	43.02814	50.01646	73.05393
228.20812	0.98461	14.02699	14.07062	15.01160	17.09336	23.03747	33.07308	42.08407	49.07239	72.10985
229.19272	**230.17733**	13.04238	13.08602	14.02699	16.10875	22.05286	32.08848	41.09946	48.08778	71.12525
242.23510	243.21971	**256.26209**	**0.04364**	0.98461	3.06637	9.01048	19.04609	28.05708	35.04540	58.08287
242.27874	243.26335	256.30573	**256.34936**	0.94097	3.02274	8.96684	19.00246	28.01345	35.00176	58.03923
243.21971	244.20432	257.24670	257.29033	**258.23131**	2.08177	8.02587	18.06149	27.07247	34.06079	57.09826
245.30148	246.28608	259.32846	259.37210	260.31307	**262.39484**	5.94411	15.97972	24.99071	31.97903	55.01649
251.24558	252.23019	265.27257	265.31621	266.25718	268.33894	**274.28305**	10.03562	19.04660	26.03492	49.07239
261.28120	262.26581	275.30819	275.35182	276.29279	278.37456	284.31867	**294.35428**	9.01099	15.99931	39.03677
270.29219	271.27679	284.31917	284.36281	285.30378	287.38555	293.32965	303.36527	**312.37625**	6.98832	30.02579
277.28050	278.26511	291.30749	291.35113	292.29210	294.37386	300.31797	310.35359	319.36457	**326.35289**	23.03747
300.31797	301.30258	314.34496	314.38859	315.32957	317.41133	323.35544	333.39105	342.40204	349.39036	**372.42783**

Sum of 2 Residues

isobaric and close-to-isobaric mass differences are color coded
isobaric and close-to-isobaric substitutions by 2 residues are color coded

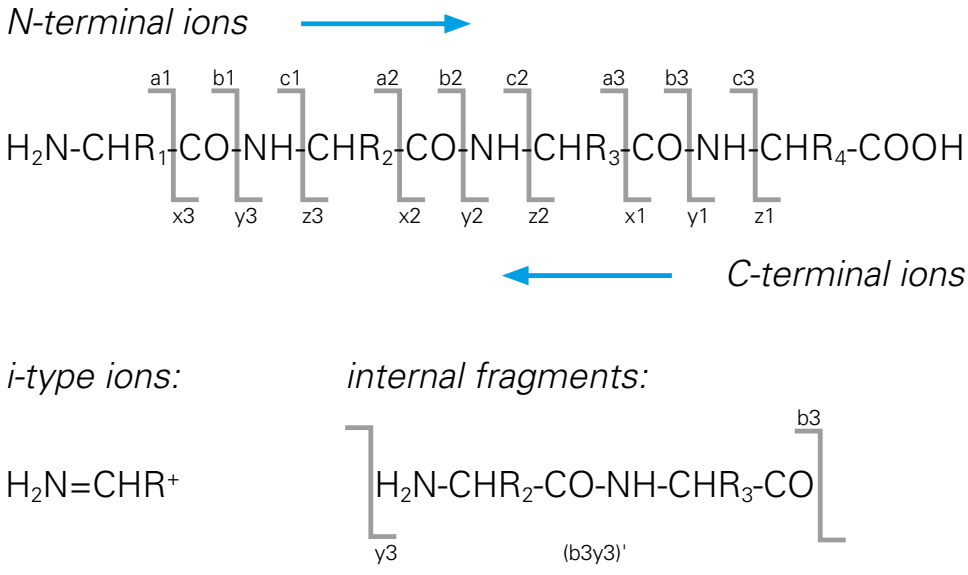
Matrices / Bruker Matrix Selection Guide

Matrix name	Elemental Composition	Structure	MH_{mono}^+ [Th]	Average Mass	Order No.
2,5-Dihydroxyacetophenon (2,5-DHAP)	$C_8H_8O_3$		153,05462	152,20	**231829**
2,5-Dihydroxybenzoic acid (2,5-DHB)	$C_7H_6O_4$		155,03388	154,12	**201346**
3-Hydroxypicolinic acid (3-HPA), 1 g	$C_6H_5NO_3$		140,03422	139,11	**201224**
α-Cyano-4-hydroxycinnamic acid (HCCA)	$C_{10}H_7NO_3$		190,04987	189,17	**201344** **255344**
super 2,5-Dihydroxybenzoic acid (sDHB), 5 g	$C_7H_6O_4$ $C_8H_8O_4$			154,12 168,15	**209813**
Sinapinic acid (SA)	$C_{11}H_{12}O_5$		225,07575	224,22	**201345**



*) http://polymers.msel.nist.gov/maldirecipes

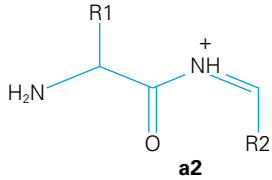
Peptide Fragmentation



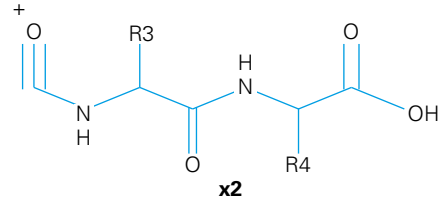
Typical fragment ions observed

- Low energy CID: b and y
- PSD: a, b, y and i, including neutral losses of NH_3 from a and b
- ISD: a, c, z+2, y
- ECD-FTICR: c and z

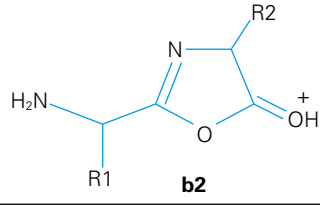
Structures of the fragments



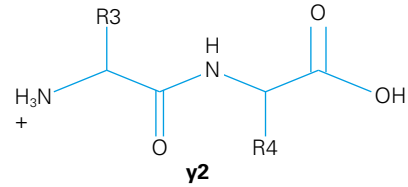
a2



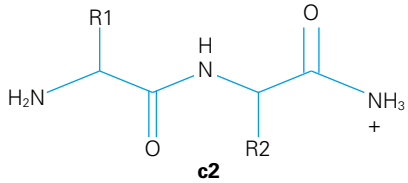
x2



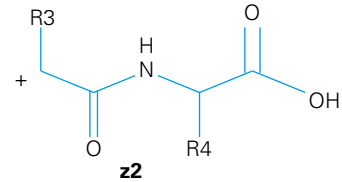
b2



y2



c2



z2

Relative Isotopic Abundance Table

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	
H	99.99	0.0115															H
He				100													He
Li						7.59	92.41										Li
Be									100								Be
B										19.9	80.1						B
C												98.93	1.07				C
N														99.64	0.36		N
O																99.76	O

	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	
O	0.04	0.21															O
F			100														F
Ne				90.48	0.27	9.25											Ne
Na							100										Na
Mg								78.99	10.00	11.01							Mg
Al											100						Al
Si												92.22	4.69	3.09			Si
P															100		P
S																94.99	S

	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	
S	0.75	4.25		0.01													S
Cl			75.76		24.24												Cl
Ar				0.34		0.06		99.60									Ar
K							93.26	0.01	6.73								K
Ca								96.94		0.647	0.135	2.086		0.004		0.187	Ca
Sc													100				Sc
Ti														8.25	7.44	73.72	Ti

	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	
Ti	5.41	5.18															Ti
V		0.25	99.75														V
Cr		4.345		83.79	9.501	2.365											Cr
Mn							100										Mn
Fe						5.845		91.75	2.11	0.28							Fe
Co											100						Co
Ni									68.08			26.22	1.14	3.63		0.93	Ni
Cu															69.15		Cu
Zn																48.27	Zn

	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	
Cu	30.85																Cu
Zn		27.98	4.10	19.02		0.63											Zn
Ga					60.11		39.89										Ga
Ge						20.38		27.31	7.76	36.72		7.83					Ge
As											100						As
Se												9.37	7.63	23.77		49.61	Se
Br															50.69		Br
Kr														0.36		2.29	Kr

	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	
Se		8.73															Se
Br	49.31																Br
Kr		11.59	11.50	56.99		17.28											Kr
Rb					72.17		27.83										Rb
Sr				0.56		9.86	7.00	82.58									Sr
Y									100								Y
Zr										51.45	11.22	17.15		17.38		2.80	Zr
Nb													100				Nb
Mo												14.77		9.23	15.90	16.68	Mo
Ru																5.54	Ru

	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	
Mo	9.56	24.19	9.67														Mo
Ru		1.87	12.76	12.60	17.06	31.55		18.62									Ru
Rh							100										Rh
Pd						1.02		11.14	22.33	27.33		26.46		11.72			Pd
Ag											51.84		48.16				Ag
Cd										1.25		0.89		12.49	12.80	24.13	Cd
Sn																0.97	Sn

Relative Isotopic Abundance Table

	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	
Cd	12.22	28.73		7.49													Cd
In	4.29		95.71														In
Sn		0.66	0.34	14.54	7.68	24.22	8.59	32.59		4.63		5.79					Sn
Sb									57.21		42.79						Sb
Te								0.09		2.55	0.89	4.74	7.07	18.84		31.74	Te
I															100		I
Xe												0.10		0.09		1.91	Xe

	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	
Te		33.8															Te
Xe	26.40	4.10	21.23	26.91		10.44		8.86									Xe
Cs					100												Cs
Ba		0.11		0.10		2.42	6.59	7.85	11.23	71.70							Ba
La										0.09	99.91						La
Ce								0.19		0.25		88.45		11.11			Ce
Pr													100				Pr
Nd														27.2	12.2	23.8	Nd
Sm																3.1	Sm

	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	
Nd	8.30	17.20		5.70		5.60											Nd
Sm			14.99	11.24	13.82	7.38		26.75		22.75							Sm
Eu							47.81		52.19								Eu
Gd								0.20		2.18	14.80	20.47	15.65	24.84		21.86	Gd
Tb															100		Tb
Dy												0.06		0.10		2.33	Dy

	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	
Dy	18.89	25.48	24.90	28.26													Dy
Ho					100												Ho
Er		0.14		1.60		33.50	22.87	26.98		14.91							Er
Tm									100								Tm
Yb								0.13		3.04	14.28	21.83	16.13	31.83		12.76	Yb
Lu															97.41	2.59	Lu
Hf														0.16		5.26	Hf

	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	
Hf	18.60	27.28	13.62	35.08													Hf
Ta				0.012	99.99												Ta
W				0.12		26.50	14.31	30.64		28.43							W
Re									37.4		62.60						Re
Os								0.02		1.59	1.96	13.24	16.15	26.26		40.78	Os
Ir															37.3		Ir
Pt														0.014		0.78	Pt

	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	
Ir	62.7																Ir
Pt		32.97	33.83	25.24		7.16											Pt
Au					100												Au
Hg				0.15		9.97	16.87	23.10	13.18	29.86		6.87					Hg
Tl											29.52		70.48				Tl
Pb												1.4		24.1	22.1	52.4	Pb

	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	
Bi	100																Bi

	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	
Th								100									Th
U										0.005	0.72			99.27			U

recommended mass number

recommended mass number for cool plasma

Molecular Weights

Molecular Weights of Selected Glycan Residues

Residue Name	Symbol	Elemental Composition	Monoisotopic Mass	Average Mass
Deoxyribose	dRib	$C_5H_8O_3$	116,04734	116,12
Arabinose	Ara	$C_5H_8O_4$	132,04226	132,11
Ribose	Rib	$C_5H_8O_4$	132,04226	132,11
Xylose	Xyl	$C_5H_8O_4$	132,04226	132,11
Fucose	Fuc	$C_6H_{10}O_4$	146,05791	146,14
Galactosamine	GalN	$C_6H_{11}NO_4$	161,06881	161,16
Glucosamin	GlcN	$C_6H_{11}NO_4$	161,06881	161,16
Galactose	Gal	$C_6H_{10}O_5$	162,05282	162,14
Glucose	Glc	$C_6H_{10}O_5$	162,05282	162,14
Mannose	Man	$C_6H_{10}O_5$	162,05282	162,14
Glucuronic acid	GlcA	$C_6H_8O_6$	176,03209	176,13
N-acetylgalactosamin	GalNAc	$C_8H_{13}NO_5$	203,07937	203,20
N-acetylglucosamin	GlcNAc	$C_8H_{13}NO_5$	203,07937	203,20
Muramic acid	Mur	$C_{11}H_{17}NO_7$	275,10050	275,26
N-acetylneuraminic acid	NANA	$C_{11}H_{17}NO_8$	291,09542	291,26

Molecular Weights of Nucleotide Residues (compatible to BioTools 3.2)

Nucleotide Residue	Elemental Composition	Monoisotopic Mass	Averaged Mass
AMP	$C_{10}H_{12}N_5O_6P$	329,05252	329,21
GMP	$C_{10}H_{12}N_5O_7P$	345,04744	345,21
UMP	$C_9H_{11}N_2O_8P$	306,02530	306,17
CMP	$C_9H_{12}N_3O_7P$	305,04129	305,18
dAMP	$C_{10}H_{12}N_5O_5P$	313,05761	313,21
dGMP	$C_{10}H_{12}N_5O_6P$	329,05252	329,21
dTMP	$C_{10}H_{13}N_2O_7P$	304,04604	304,20
dCMP	$C_9H_{12}N_3O_6P$	289,04637	289,18
Hypoxanthine	$C_{10}H_{11}N_4O_6P$	314,04162	314,19
7-deaza-dGMP	$C_{11}H_{13}N_4O_6P$	328,05727	328,22
7-deaza-dAMP	$C_{11}H_{13}N_4O_5P$	312,06236	312,22
2-amino-purine	$C_{10}H_{12}N_5O_5P$	313,05761	313,21
dAMP-thioCH3	$C_{11}H_{14}N_5O_4SP$	343,05041	343,30
dGMP-thioCH3	$C_{11}H_{14}N_5O_5SP$	359,04533	359,30
dTMP-thioCH3	$C_{11}H_{15}N_2O_6SP$	334,03885	334,29
dCMP-thioCH3	$C_{10}H_{14}N_3O_5SP$	319,03918	319,28
ddCMP	$C_9H_{12}N_3O_5P$	273,05146	273,19
ddAMP	$C_{10}H_{12}N_5O_4P$	297,06269	297,21
ddTMP	$C_{10}H_{13}N_2O_6P$	288,05112	288,20
ddGMP	$C_{10}H_{12}N_5O_5P$	313,05761	313,21

Chemical Tables

Important Abbreviations and Acronyms

A	adenine
AA	anisylacetone
AAO	acetaldehyde oxime
AC	acetate
Ac	acetyl [$CH_3C(0)–$]
acac	acetylacetone
ACTH	adrenocorticotropic hormone (corticotropin)
ADMA	alkyldimethylamine
ADP	adenosine 5′-diphosphate
AIBN	azobis(isobutyronitrile)
Ala	alanine (A)
Am	amyl
AMP	adenosine 5′-monophosphate
AN	acetonitrile
APS	adenosine 5′-phosphosulfate
Ar	aryl
Arg	arginine (R)
Asn	asparagine (N)
Asp	aspartic acid (D)
ATA	anthranilamide
ATP	adenosine 5′-triphosphate
BA	benzyladenine
BaP (BAP)	benzo[*a*]pyrene
BBP	benzyl butyl phthalate
BHC	benzene hexachloride
BHT	2,6-di-*t*-butyl-4-methylphenol
bipy	2,2'-bipyridyl
Bn	benzyl (also Bz, BZL, or Bnz)
BN	benzonitrile
Boc	t-butyloxycarbonyl
BOM	benzyloxymethyl [$PhCH_2OCH_2–$]
BON	*β*-oxynaphthoic acid
BPBG	butyl phthalyl butyl glycolate
Bs	brosylate [$BrC_6H_4SO_2–$]
BSA	*O,N*-bistrimethylsilyl acetamide
BTA	benzoyltrifluoroacetone
Bu	butyl
Bz	benzoyl
C	cytosine
p **CBA**	*p*-carboxybenzaldehyde
Cbz	carbobenzyloxy [$PhCH_2OC(O)–$]
CD	cyclodextrin
CDP	cytidine 5′-diphosphate
CE	cyanoethyl
CMP	cytidine 5′-monophosphate
CoA	coenzyme A
Cp (or cp)	cyclopentadiene
12-Crown-4	1,4,7,10-tetraoxacyclododecane
CTA	citraconic anhydride
Cys	cysteine (C)
DAA	diacetone acrylamide
DAP	dodecylammonium propionate
DCB	dicyanobenzene
DCEE	dichloroethyl ether
DDD	2,2′-dihydroxy-6,6′-dinaphthyl disulfide
DDH	1,3-dibromo-5,5-dimethylhydantoin
DDM	diphenyldiazomethane
DDT	1,1-bis(*p*-chlorophenyl)-2,2,2-trichloroethane
DEA	*N,N*-diethylaniline or diethyl amine
DEC	diethylaminoethyl chloride hydrochloride
DHA	dehydroacetic acid
DHP	dihydropyran
Diglyme	diethylene glycol dimethyl ether
Diox	dioxane
DMAc	*N,N*-dimethylacetamide
DMAA	*N,N*-dimethylacetoacetamide
DME	1,2-dimethoxyethane (glyme)
DMF	dimethylformamide
DML	dimyristoyl lecithin
DMS	dimethylsiloxane
DMSO	dimethyl sulfoxide
DMSO2	dimethyl sulfone
DMT	dimethyl terephthalate
DNA	deoxyribonucleic acid
DNF	2,4-dinitrofluorobenzene
DOCA	deoxycorticosterone acetate
DPG	2,3-diphosphoglycerate
DPL	dipalmitoyl lecithin
dpm	dipivaloylmethanato
DPPH	diphenylpicrylhydracyl
DST	disuccinimidyl tartrate
DTBN	di-t-butyl nitroxide
E	trans config. (entgegen)
EAA	ethyl acetoacetate
EAK	ethyl amyl ketone
EBA	*N*-ethyl-*N*-benzylaniline

Chemical Tables

Important Abbreviations and Acronyms

EBBA	*N*-(*p*-ethoxybenzylidene)-*p*-butylaniline
EDC	ethylene dichloride
EDTA	ethylenediaminetetraacetic acid
EGS	ethylene glycol bis(succinimidyl succinate)
en	ethylenediamine
Et	ethyl
EVA	ethylene vinyl acetate
FA	furfuryl alcohol
FAD	flavin adenine dinucleotide
FMA	fluoroscein mercuric acetate
Fmoc	9-fluorenylmethoxycarbonyl
Fuc	fucose
G	guanine
Gal	galactose
GDP	guanosine 5′-diphosphate
Glc	glucose
Gln	glutamine (Q)
Glu	glutamic acid (E)
Gly	glycine (G)
Glyme (glyme)	1,2-dimethoxyethane
HAB	4,4′-bis(heptyl)azoxybenzene
Hex	hexane (or hexyl) or hexose
HFA	hexafluoroacetone
His	histidine (H)
HMDS	hexamethyldisilazide
HMPA	hexamethylphosphoramide
HMPT	hexamethylphosphorous triamide
HOAB	*p*-*n*-heptyloxyazoxybenzene
HOAc	acetic acid
Hyp	hydroxyproline
IH	immobilized histamine
IHP	inositolhexaphosphate
Ile	isoleucine (I)
IMP	inosine 5′-monophosphate
IPN	isophthalonitrile
KDP	potassium dihydrogen phosphate
LAH	lithium aluminum hydride ($LiAlH_4$)
LAP	leucine aminopeptidase
LDH	lactic dehydrogenase
Leu	leucine (L)
Lys	lysine (K)
M	metal
MA	maleic anhydride

MAA	methoxyacetic acid
Man	mannose
MBBA	*N*-(*p*-methoxybenzylidene)-*p*-butylaniline
MCA	monochloroacetic acid
Me	methyl
MEM	β-methoxyethoxymethyl
Mes	mesityl = 2,4,6-trimethylphenyl
Met	methionine (M)
MMH	methylmercuric hydroxide
MOM	methoxymethyl
Ms	mesyl = methanesulfonyl = CH_3SO_2–
MSA	methanesulfonic acid
MTPA	α-methoxy-α-trifluoromethylphenylacetic acid
MVK	methyl vinyl ketone
NAC	*N*-acetyl
NAD(P)	nicotinamide adenine dinucleotide (phosphate)
NAD(P)H	nicotinamide adenine dinucleotide (phosphate)
NAI	*N*-acetylimidazole
NCA	*N*-chloroacetamide
Nf	nonaflate ($C_4F_9SO_2$–)
NM	nitromethane
NMA	*N*-methylacrylamide
NMF	*N*-methylformamide
Ns	*p*-nitrobenzenesulfonyl
NTA	nitrilotriacetic acid
OCBA	*o*-chlorobenzoic acid
OCT	*o*-chlorotoluene
ODCB	*o*-dichlorobenzene
P	polymer substituent
PAA	*p*-azoxyanisole
PAS	*p*-aminosalicylic acid
PBA	pyrene butyric acid
PBLG	poly(L-benzyl μ-glutamate)
PC	propylene carbonate
PCA	perchloric acid
PCB	polychlorinated biphenyl
PCP	pentachlorophenol
PDMS	poly(dimethylsiloxane)
PEG	polyethylene glycol
PET	
Ph	phenyl
Phe	phenylalanine (F)
phen	1,10-phenanthroline

Chemical Tables

Important Abbreviations and Acronyms

PMA	poly(methacrylic acid)
PMMA	poly(methyl methacrylate)
POC	cyclopentyloxycarbonyl
POM	poly(oxymethylene)
PPA	poly(phosphoric acid)
Pr	propyl
Pro	proline (P)
PS	polystyrene
PTFE	polytetrafluoroethylene
PVA	poly(vinyl alcohol)
PVC	poly(vinyl chloride)
PVF	poly(vinyl fluoride)
PVP	poly(vinyl pyrrolidone)
Pyr (or Py)	pyridine
RNA	ribonucleic acid
SDS	sodium dodecyl sulfate
Ser	serine (S)
SLS	sodium lauryl sulfate
T	thymine
TAB	trimethylammonium bromide (TMAB)
TBE	tetrabromoethane
TCA	trichloroacetic acid
TCNQ	tetracyanoquinodimethane
TEA	triethylamine
Tf	triflate [CF_3SO_2–]
TFA	trifluoroacetic acid

THF	tetrahydrofuran
THP	tetrahydropyran
Thr	threonine (T)
TIPS	triisopropylsilyl
TMB	*N,N,N′N′*-tetramethylbenzidine
TMM	trimethylenemethane
TMS	tetramethylsilyl
TMU	tetramethylurea
TNM	tetranitromethane
TNT	2,4,6-trinitrotoluene
Tol	p-tolyl
TP	thymolphthalein
TPC	thymolphthalein complexone
TPE	tetraphenylethylene
Tr	trityl = triphenylmethyl
Triglyme	triethylene glycol dimethyl ether
TRIS	tris(hydroxymethyl)aminomethane
Trp	tryptophan (W)
Ts	tosyl = *p*-toluenesulfonyl
Tyr	tyrosine (Y)
U	uracil
UTP	uridine 5′-triphosphate
Val	valine (V)
Xyl	xylose
Z	cis configuration (zusammen)

Concentration Units for Solutions

Name	Symbol	Definition
Weight percent	wt %	(Grams of solute per grams of solution) x 100
Mole fraction	X_A	Moles of A per total number of moles
Molar	*M*	Moles of solute per liter of solution
Normal	*N*	Equivalents of solute per liter of solution
Formal	*F*	Formula weights of solute per liter of solution
Molal	*m*	Moles of solute per kg of solvent
Weight formal	*f*	Formula weight of solute per kg of solvent

Acronyms and Abbreviations in Quantum Chemistry and Molecular Modeling

AEE	**A**verage **E**xcitation **E**nergy
AM1	**A**ustin **M**ethod **1**, a modified MNDO method (semi-empirical)
AMBER	**A**ssisted **M**odel **B**uilding and **E**nergy **R**efinement, P. Kollman's empirical force field for biopolymers
AMFI	**A**tomic **M**ean **FI**eld approximation for SO coupling
AO	**A**tomic **O**rbital
ARCS	**A**romatic **R**ing **C**urrent **S**hielding
BOMD	**B**orn-**O**ppenheimer **M**olecular **D**ynamics simulation
CC	**C**oupled **C**luster methods (ab initio)
CCSD(T)	**C**oupled **C**luster method at **S**ingles, **D**oubles, **T**riples level
CDFT	**C**urrent **D**ensity **F**unctional **T**heory (ab initio)
CFT	**C**rystal **F**ield **T**heory
CHARMM	**CH**emitry at **HAR**vard **M**acromolecular **M**echanics, empirical force field implementation of M. Karplus
CHF	**C**oupled **H**artree-**F**ock perturbation theory
CI	**C**onfiguration **I**nteraction
CNDO	**C**omplete **N**eglect of **D**ifferential **O**verlap (semi-empirical)
CNDO/*n*	**C**omplete **N**eglect of **D**ifferential **O**verlap (level ***n*** = 1 or 2)
CNDO/2H	CNDO/2 modified for hydrogen bonding
CPMD	**C**ar-**P**arrinello **M**olecular **D**ynamics simulation
CSGT	**C**ontinuous **S**et of **G**auge **T**ransformations (ab initio)
DFT	**D**ensity **F**unctional **T**heory (ab initio)
DFTB	**D**ensity **F**unctional **T**ight **B**inding method
DGEOM	**D**istance **GEOM**etry
DHF	relativistic four-component **D**irac-**H**artree-**F**ock method
DZ	**D**ouble **Z**eta, a basis set consisting of two STOs for each atomic orbital
EH	**E**xtended **H**ückel theory
EHT	**E**xtended **H**ückel MO **T**heory
EOM	**E**quation **O**f **M**otion
FEMO	**F**ree-**E**lectron **M**olecular **O**rbitals
FPT	**F**inite **P**erturbation **T**heory
GGA	**G**eneralized **G**radient **A**pproximation (DFT)
GIAO	**G**auge-**I**ncluding **A**tomic **O**rbitals, also used: **G**auge-**I**nvariant or **G**auge-**I**ndependent (ab initio)
GIPAW	**G**auge-**I**ncluding **P**rojector-**A**ugmented **W**aves (ab initio)
GTO	**G**aussian **T**ype atomic **O**rbital
HF	**H**artree-**F**ock method for self-consistent fields
HFC(C)	**H**yper**F**ine **C**oupling (**C**onstant)
HMO	**H**ückel **M**olecular **O**rbitals
HOMO	**H**ighest **O**ccupied **M**olecular **O**rbital
IGAIM	**I**ndividual **G**auge for **A**toms **I**n **M**olecules (ab initio)
IGLO	**I**ndividual **G**auge for **L**ocalized **O**rbitals (ab initio)
INDO	**I**ntermediate **N**eglect of **D**ifferential **O**verlap (semi-empirical)
INDO/S	**INDO** for **S**pectroscopy
JWKB	**J**effreys-**W**entzel-**K**ramers-**B**rillouin, a semiclassical approximation to quantum mechanics
K-LMG	split-valence basis set defined with K, L, M numbers of Gaussians

Acronyms and Abbreviations in Quantum Chemistry and Molecular Modeling

LCAO	**L**inear **C**ombination of **A**tomic **O**rbitals (ab initio)
LDA	**L**ocal **D**ensity **A**pproximation (DFT)
LUMO	**L**owest **U**noccupied **M**olecular **O**rbital (see HOMO)
MCSCF	**M**ulti**C**onfiguration **S**elf **C**onsistent **F**ield (ab initio)
MD	**M**olecular **D**ynamics (with any method)
MINDO	**M**odified **I**ntermediate **N**eglect to **D**ifferential **O**verlap (semi-empirical)
MINDO/*n*	**M**odified **I**ntermediate Neglect of **D**ifferential **O**verlap (***n*** = 1-3, semi-empirical)
MINDO/3H	MINDO/3 modified for hydrogen bonding
MM	**M**olecular **M**echanics (with empirical force field)
MMn	N. L. Allinger's empirical force field for small molecules (n = integer)
MNDO	**M**odified **N**eglect of **D**ifferential **O**verlap (semi-empirical)
MNDO/H	MNDO modified for hydrogen bonding
MO	**M**olecular **O**rbital
MP2	**M**øller-Plesset 2nd-order perturbation calc. (ab initio)
MR-CI	**M**ulti-**R**eference **C**onfiguration **I**nteraction
NDDO	**N**eglect of **D**iatomic **D**ifferential **O**verlap
NICS	**N**ucleus-**I**ndependent **C**hemical **S**hift (aromaticity)
OPLS	**O**ptimized **P**otentials for **L**iquid **S**imulations, W. Jorgensen's empirical force field for biopolymers
PM3	**P**arameterized **M**ethod **3** (a modification of AM1)
PPP	**P**ariser-**P**arr-**P**ople method (semi-empirical)
QSAR	**Q**uantitative **S**tructure-Activity **R**elationship
REX	**R**elativistic **EX**tended Hückel MOs
RHF	**R**estricted **H**artee-**F**ock method (for SCF calculations)
SCF	**S**elf-**C**onsistent **F**ield
SCPT	**S**elf-**C**onsistent **P**erturbation **T**heory
SCRF	**S**elf-**C**onsistent **R**eaction **F**ield for free radicals
SD	**S**pin-**D**ipolar term
SO	**S**pin-**O**rbit coupling
SOMO	**S**ingly **O**ccupied **M**olecular **O**rbital
SOS	**S**um **O**ver **S**tates perturbation theory
STO	**S**later **T**ype **O**rbital basis set (ab initio)
STO-*n*G	**S**later **T**ype **O**rbitals as a sum of *n* Gaussians
TFD	**T**homas-**F**ermi-**D**irac method, a statistical treatment of electron density
UCHF	**U**n**C**oupled **H**artree-**F**ock perturbation method
UHF	**U**nrestricted **H**artee-**F**ock method for SCF calculations
VB	**V**alence **B**ond theory
VSEPR	**V**alence-**S**hell **E**lectron **P**air **R**epulsion, a theory of molecular geometry
VWN	**V**osko, **W**ilk, **N**usair parameterization for LDA
WKB	**W**entzel-**K**ramers-**B**rillouin method, a semiclassical approximation to quantum mechanics
ZDO	**Z**ero **D**ifferential **O**verlap (semi-empirical)
ZFS	**Z**ero-**F**ield **S**plitting
ZINDO	**Z**erner's **INDO** method
ZORA	**Z**ero-**O**rder **R**egular **A**pproximatio

IUPAC Periodic Table of Elements

BRUKER

1 (IA)	2 (IIA)	3 (IIIB)	4 (IVB)	5 (VB)	6 (VIB)	7 (VIIB)	8 (VIII)	9 (VIII)
Hydrogen 1 **H_1** -259.34° -252.87° -240.18° +1-1 1.00794 91.0%								
Lithium 2 1 **Li_3** 180.5° 1342° +1 6.941 $1.86 \cdot 10^{-7}$%	**Beryllium** 2 2 **Be_4** 1287° 2471° +2 9.012182 $2.38 \cdot 10^{-9}$%							
Sodium 2 8 1 **Na_{11}** 97.80° 883° +1 22.98976928 0.000187%	**Magnesium** 2 8 2 **Mg_{12}** 650° 1090° +2 24.3050 0.00350%							
Potassium 2 8 8 1 **K_{19}** 63.38° 759° +1 39.0983 0.0000123%	**Calcium** 2 8 8 2 **Ca_{20}** 842° 1484° +2 40.078 0.000199%	**Scandium** 2 8 9 2 **Sc_{21}** 1541° 2836° +3 44.955912 $1.12 \cdot 10^{-7}$%	**Titanium** 2 8 10 2 **Ti_{22}** 1668° 3287° +2+3+4 47.867 $7.8 \cdot 10^{-6}$%	**Vanadium** 2 8 11 2 **V_{23}** 1910° 3407° +2+3+4+5 50.9415 $9.6 \cdot 10^{-7}$%	**Chromium** 2 8 13 1 **Cr_{24}** 1907° 2671° +2+3+6 51.9961 0.000044%	**Manganese** 2 8 13 2 **Mn_{25}** 1246° 2061° +2+3+4+7 54.938045 0.000031%	**Iron** 2 8 14 2 **Fe_{26}** 1538° 2861° +2+3 55.845 0.00294%	**Cobalt** 2 8 15 2 **Co_{27}** 1495° 2927° +2+3 58.933195 $7.3 \cdot 10^{-6}$%
Rubidium 2 8 18 8 1 **Rb_{37}** 39.31° 688° +1 85.4678 $2.31 \cdot 10^{-8}$%	**Strontium** 2 8 18 8 2 **Sr_{38}** 777° 1382° +2 87.62 $7.7 \cdot 10^{-8}$%	**Yttrium** 2 8 18 9 2 **Y_{39}** 1522° 3345° +3 88.90585 $1.51 \cdot 10^{-8}$%	**Zirconium** 2 8 18 10 2 **Zr_{40}** 1855° 4409° +4 91.224 $3.72 \cdot 10^{-8}$%	**Niobium** 2 8 18 12 1 **Nb_{41}** 2477° 4744° +3+5 92.90638 $2.28 \cdot 10^{-9}$%	**Molybdenum** 2 8 18 13 1 **Mo_{42}** 2623° 4639° +6 95.96 $8.3 \cdot 10^{-9}$%	**Technetium** 2 8 18 13 2 **Tc_{43}** 2157° 4265° +4+6+7 [98]	**Ruthenium** 2 8 18 15 1 **Ru_{44}** 2334° 4150° +3 101.07 $6.1 \cdot 10^{-9}$%	**Rhodium** 2 8 18 16 1 **Rh_{45}** 1964° 3695° +3 102.90550 $1.12 \cdot 10^{-9}$%
Cesium 2 8 18 18 8 1 **Cs_{55}** 28.44° 671° +1 132.9054519 $1.21 \cdot 10^{-9}$%	**Barium** 2 8 18 18 8 2 **Ba_{56}** 727° 1897° +2 137.327 $1.46 \cdot 10^{-8}$%	**Lanthanum** 2 8 18 18 9 2 **La_{57}** † 918° 3464° +3 138.90547 $1.45 \cdot 10^{-9}$%	**Hafnium** 2 8 18 32 10 2 **Hf_{72}** 2233° 4603° +4 178.49 $5.02 \cdot 10^{-10}$%	**Tantalum** 2 8 18 32 11 2 **Ta_{73}** 3017° 5458° +5 180.94788 $6.75 \cdot 10^{-11}$%	**Tungsten** 2 8 18 32 12 2 **W_{74}** 3422° 5555° +6 183.84 $4.34 \cdot 10^{-10}$%	**Rhenium** 2 8 18 32 13 2 **Re_{75}** 3186° 5596° +4+6+7 186.207 $1.69 \cdot 10^{-10}$%	**Osmium** 2 8 18 32 14 2 **Os_{76}** 3033° 5012° +3+4 190.23 $2.20 \cdot 10^{-9}$%	**Iridium** 2 8 18 32 15 2 **Ir_{77}** 2446° 4428° +3+4 192.217 $2.16 \cdot 10^{-9}$%
Francium 2 8 18 32 18 8 1 **Fr_{87}** 27° +1 [223]	**Radium** 2 8 18 32 18 8 2 **Ra_{88}** 700° +2 [226]	**Actinium** 2 8 18 32 18 9 2 **Ac_{89}** ‡ 1051° 3198° +3 [227]	**Rutherfordium** 2 8 18 32 32 10 2 **Rf_{104}** +4 [267]	**Dubnium** 2 8 18 32 32 11 2 **Db_{105}** [268]	**Seaborgium** 2 8 18 32 32 12 2 **Sg_{106}** [271]	**Bohrium** 2 8 18 32 32 13 2 **Bh_{107}** [272]	**Hassium** 2 8 18 32 32 14 2 **Hs_{108}** [277]	**Meitnerium** 2 8 18 32 32 15 2 **Mt_{109}** [276]

Group

Element
K **E_Z** M.P.°
L B.P.°
M C.P.°
N Ox.States
O At.Weight
P
Q Abundance%

Key to Table

† Lanthanides	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium
	2 8 18 19 9 2 **Ce_{58}** 798° 3443° +3+4 140.116 $3.70 \cdot 10^{-9}$%	2 8 18 21 8 2 **Pr_{59}** 931° 3520° +3 140.90765 $5.44 \cdot 10^{-10}$%	2 8 18 22 8 2 **Nd_{60}** 1021° 3074° +3 144.242 $2.70 \cdot 10^{-9}$%	2 8 18 23 8 2 **Pm_{61}** 1042° 3000° +3 [145]	2 8 18 24 8 2 **Sm_{62}** 1074° 1794° +2+3 150.36 $8.42 \cdot 10^{-10}$%	2 8 18 25 8 2 **Eu_{63}** 822° 1596° +2+3 151.964 $3.17 \cdot 10^{-10}$%	2 8 18 25 9 2 **Gd_{64}** 1313° 3273° +3 157.25 $1.076 \cdot 10^{-9}$%

‡ Actinides	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium
	2 8 18 32 18 10 2 **Th_{90}** 1750° 4788° +4 232.03806 $1.09 \cdot 10^{-10}$%	2 8 18 32 20 9 2 **Pa_{91}** 1572° +5+4 231.03588	2 8 18 32 21 9 2 **U_{92}** 1135° 4131° +3+4+5+6 238.02891 $2.94 \cdot 10^{-11}$%	2 8 18 32 22 9 2 **Np_{93}** 644° +3+4+5+6 [237]	2 8 18 32 24 8 2 **Pu_{94}** 640° 3228° +3+4+5+6 [244]	2 8 18 32 25 8 2 **Am_{95}** 1176° 2011° +3+4+5+6 [243]	2 8 18 32 25 9 2 **Cm_{96}** 1345° +3 [247]

Key to Table: The IUPAC Group Numbers 1 to 18 are used (CAS group numbering in parentheses). Information presented: E_Z = element symbol and nuclear charge (protons); melting, boiling, critical point (MP, BP, CP) in °C (sublimation or critical temp. marked with s or t); population of electron levels K - Q; possible oxidation states; **IUPAC mean atomic weights updated 2005** based on terrestrial isotope abundances (^{12}C = 12.0000); for unnatural elements atom. wt. of most abundant isotope is given in brackets; total element abundance (%) in the solar system.

18 (VIIIA)	13 (IIIA)	14 (IVA)	15 (VA)	16 (VIA)	17 (VIIA)	
Helium	**Boron**	**Carbon**	**Nitrogen**	**Oxygen**	**Fluorine**	
2 He_2 -272.2° -268.93° -267.96° 0 4.002602 8.9%	2 3 B_5 2075° 4000° +3 10.811 6.9· 10^{-8}%	2 4 C_6 4492t° 3642s° +2+4-4 12.0107 0.033%	2 5 N_7 -210.00° -195.79° -146.94° ±1±2±3+4+5 14.0067 0.0102%	2 6 O_8 -218.79° -182.95° -118.56° -2 15.9994 0.078%	2 7 F_9 -219.62° -188.12° -129.02° -1 18.9984032 2.7· 10^{-6}%	
Neon	**Aluminum**	**Silicon**	**Phosphorus**	**Sulfur**	**Chlorine**	**Argon**
2 8 Ne_{10} -248.59° -246.08° -228.7° 0 20.1797 0.0112%	2 8 3 Al_{13} 660.32° 2519° +3 26.9815386 0.000277%	2 8 4 Si_{14} 1414° 3265° +2+4-4 28.0855 0.00326%	2 8 5 P_{15} 44.15° 280.5° 721° +3+5-3 30.973762 0.000034%	2 8 6 S_{16} 115.21° 444.60° 1041° +4+6-2 32.065 0.00168%	2 8 7 Cl_{17} -101.5° -34.04° 143.8° +1+5+7-1 35.453 0.000017%	2 8 8 Ar_{18} -189.35° -185.85° -122.28° 0 39.948 0.000329%

10 (VIII)	11 (IB)	12 (IIB)						
Nickel	**Copper**	**Zinc**	**Gallium**	**Germanium**	**Arsenic**	**Selenium**	**Bromine**	**Krypton**
2 8 16 2 Ni_{28} 1455° 2913° +2+3 58.6934 0.000161%	2 8 18 1 Cu_{29} 1084.62° 2562° +1+2 63.546 1.70· 10^{-6}%	2 8 18 2 Zn_{30} 419.53° 907° +2 65.38 4.11· 10^{-6}%	2 8 18 3 Ga_{31} 29.76° 2204° +3 69.723 1.23· 10^{-7}%	2 8 18 4 Ge_{32} 938.25° 2833° +2+4 72.64 3.9· 10^{-7}%	2 8 18 5 As_{33} 817t° 614s° 1400° +3+5-3 74.92160 2.1· 10^{-8}%	2 8 18 6 Se_{34} 221° 685° 1493° +4+6-2 78.96 2.03· 10^{-7}%	2 8 18 7 Br_{35} -7.2° 58.8° 315° +1+5-1 79.904 3.8· 10^{-8}%	2 8 18 8 Kr_{36} -157.36° -153.22° -63.74° 0 83.798 1.5· 10^{-7}%
Palladium	**Silver**	**Cadmium**	**Indium**	**Tin**	**Antimony**	**Tellurium**	**Iodine**	**Xenon**
2 8 18 18 0 Pd_{46} 1554.9° 2963° +2+4 106.42 4.5· 10^{-9}%	2 8 18 18 1 Ag_{47} 961.78° 2162° +1 107.8682 1.58· 10^{-9}%	2 8 18 18 2 Cd_{48} 321.07° 767° +2 112.411 5.3· 10^{-9}%	2 8 18 18 3 In_{49} 156.60° 2072° +3 114.818 6.0· 10^{-10}%	2 8 18 18 4 Sn_{50} 231.93° 2602° +2+4 118.710 1.25· 10^{-8}%	2 8 18 18 5 Sb_{51} 630.63° 1587° +3+5-3 121.760 1.01· 10^{-9}%	2 8 18 18 6 Te_{52} 449.51° 988° +4+6-2 127.60 1.57· 10^{-8}%	2 8 18 18 7 I_{53} 113.7° 184.4° 546° +1+5+7-1 126.90447 2.9· 10^{-9}%	2 8 18 18 8 Xe_{54} -111.75° -108.04° 16.58° 0 131.293 1.5· 10^{-8}%
Platinum	**Gold**	**Mercury**	**Thallium**	**Lead**	**Bismuth**	**Polonium**	**Astatine**	**Radon**
2 8 18 32 16 2 Pt_{78} 1768.4° 3825° +2+4 195.084 4.4· 10^{-9}%	2 8 18 32 18 1 Au_{79} 1064.18° 2856° +1+3 196.966569 6.1· 10^{-10}%	2 8 18 32 18 2 Hg_{80} -38.83° 356.73° 1477° +1+2 200.59 1.11· 10^{-9}%	2 8 18 32 18 3 Tl_{81} 304° 1473° +1+3 204.3833 6.0· 10^{-10}%	2 8 18 32 18 4 Pb_{82} 327.46° 1749° +2+4 207.2 1.03· 10^{-8}%	2 8 18 32 18 5 Bi_{83} 271.40° 1564° +3+5 208.98040 4.7· 10^{-10}%	2 8 18 32 18 6 Po_{84} 254° 962° +2+4 [209]	2 8 18 32 18 7 At_{85} 302° [210]	2 8 18 32 18 8 Rn_{86} -71° -61.7° 104° 0 [222]
Darmstadtium	**Roentgenium**	**Copernicium**						
2 8 18 32 32 16 2 Ds_{110} [281]	2 8 18 32 32 17 2 Rg_{111} [280]	2 8 18 32 32 18 2 Cn_{112} [285]						

Terbium	**Dysprosium**	**Holmium**	**Erbium**	**Thulium**	**Ytterbium**	**Lutetium**
2 8 18 27 8 2 Tb_{65} 1356° 3230° +3 158.92535 1.97· 10^{-10}%	2 8 18 28 8 2 Dy_{66} 1412° 2567° +3 162.500 1.286· 10^{-9}%	2 8 18 29 8 2 Ho_{67} 1474° 2700° +3 164.93032 2.90· 10^{-10}%	2 8 18 30 8 2 Er_{68} 1529° 2868° +3 167.259 8.18· 10^{-10}%	2 8 18 31 8 2 Tm_{69} 1545° 1950° +3 168.93421 1.23· 10^{-10}%	2 8 18 32 8 2 Yb_{70} 819° 1196° +2+3 173.054 8.08· 10^{-10}%	2 8 18 32 9 2 Lu_{71} 1663° 3402° +3 174.9668 1.197· 10^{-10}%

Berkelium	**Californium**	**Einsteinium**	**Fermium**	**Mendelevium**	**Nobelium**	**Lawrencium**
2 8 18 32 27 8 2 Bk_{97} 1050° +3+4 [247]	2 8 18 32 28 8 2 Cf_{98} 900° +3 [251]	2 8 18 32 29 8 2 Es_{99} 860° +3 [252]	2 8 18 32 30 8 2 Fm_{100} 1527° +3 [257]	2 8 18 32 31 8 2 Md_{101} 827° +2+3 [258]	2 8 18 32 32 8 2 No_{102} 827° +2+3 [259]	2 8 18 32 32 9 2 Lr_{103} 1627° +3 [262]

Adapted by W. E. Hull from the Table prepared by Richard B. Firestone (rbf@lbl.gov), Isotopes Project, Lawrence Berkeley National Laboratory; see R. B. Firestone, C. M. Baglin, and S.Y. F. Chu, 1999 Update to the 8th Edition of the *Table of Isotopes*, John Wiley & Sons, (1999); for Atomic Wt. updates see T. B. Coplen, Pure Appl Chem 73 (2001) 667-683 and R. D. Loss, Pure Appl Chem 75 (2003) 1107-1122.

Properties of Selected Nondeuterated Solvents

Solvent	Formula	MW_{ave}	Density d_4^{20} [g/mL]	Viscosity η^{25} [mPa•s, cP]	MP [°C]	BP [°C]	Refrac. Index n_D^{20}	Dielec. Const. ε	Dipole Mom. [*D*]	Chemical Shift δ_H (ppm)	Chemical Shift δ_C (ppm)
Acetic acid	$C_2H_4O_2$	60.05	1.049	1.13	16.5	118.1	1.3716	6.17	1.7	2.10 11.42	20.8 178.1
Acetone	C_3H_6O	58.08	0.788	0.306	–94.5	56.2	1.3587	20.7	2.8	2.05	30.50 205.4
Acetonitrile	C_2H_3N	41.05	0.784	0.35	–45.2	81.7	1.3441	37.5	3.44	1.93	1.6 117.8
Benzene	C_6H_6	78.11	0.8789	0.604	5.5	80.2	1.5011	2.29	0	7.16	128.5
1-Butanol	$C_4H_{10}O$	74.12	0.8097	2.55	–89.5	117.6	1.3993	17.7	1.70	1.0-1.5 3.5	14, 19 34, 63
2-Butanone (methyl ethyl ketone)	C_4H_8O	72.11	0.805	0.378	–86.7	79.6	1.3788	18.5	2.77	1.1, 2.2 2.5	7, 27.5 35, 207
Carbon disulfide	CS_2	76.14	1.270	0.363	–111.8	46.1	1.628	2.6	0		192.8
Carbon tetrachloride	CCl_4	153.82	1.590	0.908	–22.9	76.7	1.460	2.22	0		96.7
Chloroform	$CHCl_3$	119.38	1.480	0.537	–63.5	61.2	1.4458	4.81	1.08	7.26	77.2
Chloromethane	CH_3Cl	50.49	0.916	0.24	–97.5	–24.1	1.3389	12.6	1.87	3.06	25.6
Cyclohexane	C_6H_{12}	84.16	0.7786	0.894	6.5	80.8	1.4262	2.02	0	1.4	27.6
Cyclopentane	C_5H_{10}	70.13	0.745	0.44	–94.0	49.3	1.4065	1.94	0	1.5	26.5
Dibromomethane	CH_2Br_2	173.84	2.485		–52.7	96.9	1.5419	7.5	1.43	5.0	21.6
o-Dichlorobenzene	$C_6H_4Cl_2$	147.00	1.31	1.324	–17.2	180.3	1.5515	9.9	2.27	7.0-7.4	128-133
1,2-Dichloroethane	$C_2H_4Cl_2$	98.96	1.253	0.79	–35.7	83.4	1.4448	10.4	1.83	3.7	51.7
cis-1,2-Dichloroethylene	$C_2H_2Cl_2$	96.94	1.284		–80.0	60.6	1.4490	9.2	1.90	6.4	119.3
trans-1,2-Dichloroethylene	$C_2H_2Cl_2$	96.94	1.257		–49.8	47.7	1.4462	2.1	0	6.3	121.1
1,1-Dichloroethylene	$C_2H_2Cl_2$	96.94	1.213		–122.6	31.6	1.4254	4.6	1.34	5.5	115.5 128.9
Dichloromethane	CH_2Cl_2	84.93	1.326	0.41	–96.7	39.9	1.424	9.0	1.60	5.31	53.73
Diethylether	$C_4H_{10}O$	74.12	0.713	0.230	–116.3	34.6	1.3526	4.30	1.25	1.2 3.5	17.1 67.4
Diethylene glycol dimethyl ether (diglyme)	$C_6H_{14}O_3$	134.18	0.947	0.989	–64.1	162.0	1.407	7.1		3.3-3.6	59.0 70.5 72
1,2-Dimethoxyethane (glyme)	$C_4H_{10}O_2$	90.12	0.868	0.46	–69 –58	85	1.379	7.20	1.71	3.3 3.5	59 72
Dimethoxymethane	$C_3H_8O_2$	76.10	0.866		–105.2	42.3	1.3563	2.6		3.3 4.4	54.8 97.9
N,N-Dimethylacetamide	$C_4H_9N_O$	87.12	0.9415	2.14	–20	166	1.437	37.8	3.75	2.1 3	21.5 34, 38 169.6
Dimethylcarbonate	$C_3H_6O_3$	90.08	1.069		3	90.5	1.3688			3.65	54.8 156.9
Dimethylether	C_2H_6O	46.07			–139	–24.5				1.3	59.4
N,N-Dimethyl-formamide	C3H7NO	73.10	0.9487	0.92	–60.5	152.9	1.4305	36.7	3.86	2.8 2.9 8.0	30.10 35.2 162.5
Dimethylsulfoxide	C_2H_6OS	78.14	1.100	1.987	18.5	189.5	1.4783	46.7	4.0	2.49	39.50
1,4-Dioxane	$C_4H_8O_2$	88.11	1.034	1.18	11.9	101.2	1.4224	2.25	0.45	3.53	67.30
Ethanol	C_2H_6O	46.07	0.789	1.074	–114.4	78.4	1.3614	24.5	1.69	1.10	17.20 56.70
Ethyl acetate	$C_4H_8O_2$	88.11	0.896	0.426	–83.8	77.1	1.3724	6.0	1.8	1.2 2.0 4.1	14.3 20.7 60.1 170.4
Ethylene carbonate	$C_3H_4O_3$	88.06	1.321	1.93	36.4	244	1.416	89.6	4.91	4.2	65.0 155.8
Ethylene glycol	$C_2H_6O_2$	62.07	1.115	21 (20 °C)	–12.6	197.5	1.431	37.7		3.7	63.4
Formamide	CH_3NO	45.04	1.133	3.3	2.6	210.5	1.4475	110	3.38	7.2 8.1	165.1
Glycerol	$C_3H_8O_3$	92.10	1.26	940	17.9	290.1	1.474	42.5		3.4 3.7	64.5 73.7

Properties of Selected Nondeuterated Solvents

Solvent	Formula	MW_{ave}	Density d_4^{20} [g/mL]	Viscosity η^{25} [mPa•s, cP]	MP [°C]	BP [°C]	Refrac. Index n_D^{20}	Dielec. Const. ε	Dipole Mom. [*D*]	Chemical Shift δ_H (ppm)	Chemical Shift δ_C (ppm)
Hexamethyl-phosphoramide (HMPA)	$C_6H_{18}N_3OP$	179.20	1.027		7.2	233	1.4588	30.6	5.5	2.4 2.6	36.6
Hexane	C_6H_{14}	86.18	0.6594	0.294	–95.4	68.8	1.3749	1.89	0.08		
Methanesulfonic acid	CH_4O_3S	96.11	1.48	10.52	18	168	1.430			2.8	39.6
Methanol	CH_4O	32.04	0.791	0.544	–97.7	64.7	1.3284	32.6	1.70	3.31	49.0
Morpholine	C_4H_9NO	87.12	1.005	2.011	–3.1	128.9	1.4548	7.4	1.58	2.6 3.9	46.8 68.9
Nitromethane	CH_3NO_2	61.04	1.137	0.61	–28.7	100.9	1.3817	35.9	3.46	4.33	62.8
Pentane	C_5H_{12}	72.15	0.626	0.224	–129.7	36.1	1.3575	1.84	0.04		
2-Propanol	C_3H_8O	60.10	0.786	2.1	–87.9	82.4	1.3772	19	1.66	1.2 3.4	25.3 64.0
Pyridine	C_5H_5N	79.10	0.983	0.95	–41.8	115.4	1.510	12.4	2.3	7.21 7.57 8.72	123.5 135.5 149.5
Quinoline	C_9H_7N	129.16	1.098		–14.9	237.7	1.6293	9.0	2.2	7-8.8	121-151
1,1,2,2-Tetrachloroethane	$C_2H_2Cl_4$	167.85	1.60	1.58	–43.5	146.2	1.486	8.2	1.3	6.0	74.0
Tetrachloroethylene	C_2Cl_4	165.83	1.622	0.89	–22.2	121.1	1.504	2.3			120.4
Tetrahydrofuran	C_4H_8O	72.11	0.889	0.46	–108.6	66.0	1.407	7.5	1.68	1.72 3.57	25.26 67.2
Toluene	C_7H_8	92.14	0.867	0.56	–95.0	110.7	1.4969	2.38	0.36	2.09 7.01 7.09	21.3 138.5
Trichloroethylene	C_2HCl_3	131.39	1.465	0.545	–84.7	87.1	1.4767	3.4	0.81	6.4	116.7 124.0
Triethylamine	$C_6H_{15}N$	101.19	0.728	0.363	–114.7	89.2	1.401	2.42	0.87	1.0, 2.5	13, 51
Trifluoroacetic acid	$C_2HF_3O_2$	114.02	1.53	1.14	–15.4	72.5	1.285	42.1	2.26		115.7 163.8
2,2,2-Trifluoroethanol	$C_2H_3F_3O$	100.04	1.384	1.76	–44	74	1.291	8.55	2.52	3.9 5.0	62 126.3
Water	H_2O	18.02	0.9982	0.8909	0.0	100.0	1.3329	80.1	1.85	4.72	
o-Xylene	C_8H_{10}	106.17	0.88	0.76	–25.2	144.5	1.505	2.57	0.5	2.4 6.9	18 125-137

Data were revised 2006 from a variety of sources; density and refractive index are at 20°C, other parameters mainly at 25°C; exceptions occur when the solvent is not liquid at these temperatures; MP and BP are means or best values from the NIST Chem WebBook.

Electronegativities according to Pauling

Main group elements						
H 2.20						
Li 0.98	Be 1.57	B 2.04	C 2.55	N 3.04	O 3.44	F 3.98
Na 0.93	Mg 1.31	Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16
K 0.82	Ca 1.10	Ga 2.01	Ge 2.01	As 2.18	Se 2.55	Br 2.96
Rb 0.82	Sr 0.95	In 1.78	Sn 1.96	Sb 2.05	Tr 2.1	I 2.66
Cs 0.7	Ba 0.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2

d-block elements									
Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6
Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7
La 1.1	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9

f-block elements
All 1.1-1.3

Physical Tables

Fundamental Physical Constants (CODATA 2010) [a]

Quantity	Symbol	SI Value
Speed of Light (vacuum)	c, c_o	2.997 924 58 × 10^{8} m s^{-1} (defined)
Permeability of vacuum	μ_0	4π × 10^{-7} H m^{-1} or N A^{-2} (defined)
Permittivity of vacuum	$\varepsilon_0 = 1/(\mu_0 c_0^2)$	8.854 187 817 .... × 10^{-12} F m^{-1} (defined)
Planck Constant	h	6.626 069 57 (29) × 10^{-34} J s
	$\hbar = h / 2\pi$ (au)	1.0544 571 726 (47) × 10^{-34} J s
Elementary Charge (au)	e	1.602 176 565 (35) × 10^{-19} C
Electron Rest Mass (au)	m_e	9.109 382 91 (40) × 10^{-31} kg
Proton Rest Mass	m_p	1.672 621 777 (74) × 10^{-27} kg
Proton/Electron Mass Ratio	m_p / m_e	1836.152 672 45 (75)
Neutron Rest Mass	m_n	1.674 927 351 (74) × 10^{-27} kg
Deuteron Rest Mass	m_d	3.343 583 48 (15) × 10^{-27} kg
Atomic Mass Unit (^{12}C/12)	m_u = 1 u = 1 Da	1.660 538 921 (73) × 10^{-27} kg
Avogadro's Number	N_A	6.022 141 29 (27) × 10^{23} mol^{-1}
Boltzmann Constant	k	1.380 6488 (13) × 10^{-23} J K^{-1}
Faraday Constant	F	9.648 533 65 (21) × 10^{4} C mol^{-1}
Gas Constant	R	8.314 4621 (75) J mol^{-1} K^{-1}
Molar Volume of ideal gas [b]	$V_m = RT/p$	22.413 968 (20) × 10^{-3} m^3 mol^{-1}
Standard Atmosphere	atm	101.325 kPa (defined)
Fine Structure Constant	$\alpha = \mu_0 e^2 c_0 / 2h$	7.297 352 5698 (24) × 10^{-3}
Inverse Fine-Structure Constant	$1/\alpha$	137.035 999 074 (44)
Bohr Radius (au)	$a_0 = 4\pi\varepsilon_0\hbar^2 / m_e e^2$	0.529 177 210 92 (17) × 10^{-10} m
Hartree Energy (au)	$E_h = \hbar^2 / m_e a_0^2$	4.359 744 34 (19) × 10^{-18} J
Rydberg Constant	$R_\infty = E_h / 2hc_0$	10.973 731 568 539 (55) × 10^{7} m^{-1}
Compton Wavelength (Electron)	$\lambda_C = h / m_e c_0$	2.426 310 2389 (16) × 10^{-12} m
Bohr Magneton (β, β_e)	$\mu_B = e\hbar / 2m_e$	927.400 968 (20) × 10^{-24} J T^{-1}
Electron Magnetic Moment	μ_e	–928.476 430 (21) × 10^{-26} J T^{-1}
Electron Magnetogyric Ratio	$\gamma_e = 2\mu_e / \hbar$	1.760 859 708 (39) × 10^{11} s^{-1} T^{-1}
	$\gamma_e / 2\pi$	28.024 952 66 (62) GHz T^{-1}
Free Electron Landé g factor	$g_e = 2\mu_e / \mu_B$	–2.002 319 304 361 53 (53)
Nuclear Magneton (β_N)	$\mu_N = (m_e / m_p)\ \mu_B$	5.050 783 53 (11) × 10^{-27} J T^{-1}
Proton Magnetic Moment (free)	μ_p	1.410 606 743 (33) × 10^{-26} J T^{-1}
(shielded, H_2O sphere, 25°C)	μ_p'	1.410 570 499 (35) × 10^{-26} J T^{-1}
Proton Magnetogyric Ratio (free)	γ_p	2.675 222 005 (63) × 10^{8} s^{-1} T^{-1}
(shielded, H_2O sphere, 25°C)	γ_p'	2.675 153 268 (66) × 10^{8} s^{-1} T^{-1}
Proton MR freq. in H_2O	$\gamma_p' / 2\pi$	42.576 3866 (10) MHz T^{-1}
Electron/Proton Magn. Mom. Ratio	μ_e / μ_p	–658.210 6848 (54)
Deuteron Magnetic Moment	μ_d	0.433 073 489 (10) × 10^{-26} J T^{-1}
Gravitation Constant (Newtonian)	G	6.673 84 (80) × 10^{-11} m^3 kg^{-1} s^{-2}
Standard Acceleration (Earth gravity)	g_n	9.806 65 m s^{-2} (defined)
π = 3.141 592 653 59	e = 2.7180281 828 46	ln 10 = 2.302 585 092 99

[a] au = atomic units; uncertainty of last digits shown in ( ); source: http://physics.nist.gov/constants
[b] at STP of 273.15 K and 101.325 kPa = 1 atm.

Physical Tables

SI Unit System (Système International) adapted from NIST Publication 330 (2001)

Fundamental SI Base Units	Unit Name	Symbol
length (l, λ)	meter	m
mass (m)	kilogram	kg
time (t)	second	s
electric current (I)	ampere	A
thermodynamic temperature (T)	kelvin	K
amount of substance (n)	mole	mol
luminous intensity (I_v)	candela	cd
SI-derived Quantities	**Unit Name**	**Symbol**
area (A)	square meter	m^2
volume (V)	cubic meter	m^3
speed, velocity ($\boldsymbol{v}$)	meter per second	m/s
acceleration ($\boldsymbol{a}$)	meter per second squared	m/s^2
momentum ($\boldsymbol{p} = m\boldsymbol{v}$)	kilogram meter per second	kg m/s
moment or inertia (I, J)	kilogram square meter	kg m^2
mass density (ρ)	kilogram per cubic meter	kg/m^3
specific volume (v)	cubic meter per kilogram	m^3/kg
molar mass (M)	kg per mole	kg/mol
molar volume (V_m)	cubic meter per mole	m^3/mol
concentration (c)	mole per cubic meter	mol/m^3
molal concentration (m)	mole per kilogram	mol/kg
kinematic viscosity (ν) diffusion coefficient (D)	square meter per second	m^2/s
electric current density (J)	ampere per square meter	A/m^2
magnetic field strength ($\boldsymbol{H}$) magnetization ($\boldsymbol{M} = \boldsymbol{B}/\mu_0 - \boldsymbol{H}$)	ampere per meter	A/m
magnetic dipole moment ($\boldsymbol{m}$, $\boldsymbol{\mu}$)	ampere square meter	A m^2
wave number ($\tilde{\nu}$)	reciprocal meter	m^{-1}
luminance (L_v)	candela per square meter	cd/m^2
refractive index (n)	(dimensionless)	

SI Prefix	Symbol	Factor
yocto	y	10^{-24}
zepto	z	10^{-21}
atto	a	10^{-18}
femto	f	10^{-15}
pico	p	10^{-12}
nano	n	10^{-9}
micro	μ	10^{-6}
milli	m	10^{-3}
centi	c	10^{-2}
deci	d	10^{-1}
deka	da	10^{1}
hecto	h	10^{2}
kilo	k	10^{3}
mega	M	10^{6}
giga	G	10^{9}
tera	T	10^{12}
peta	P	10^{15}
exa	E	10^{18}
zetta	Z	10^{21}
yotta	Y	10^{24}

Special SI-derived Quantities	Unit Name	Symbol	SI-derived and Base Units
plane angle ($\alpha = s/r$)	radian	rad	$m\ m^{-1} = 1$ [2π rad = 360°], 1 rad = 57.2957795°
solid angle ($\Omega = A/r^2$)	steradian	sr	$m^2\ m^{-2} = 1$ [4π sr = sphere]
frequency (ν , f)	hertz	Hz	s^{-1}
force ($\boldsymbol{F} = m\boldsymbol{a}$)	newton	N	m kg s^{-2}
pressure, stress (p, P, $\sigma = \boldsymbol{F}/A$)	pascal	Pa	$N/m^2 = m^{-1}$ kg s^{-2}
energy, work, heat (E, W)	joule	J	N m = m^2 kg s^{-2}
power, radiant flux (P)	watt	W	J/s = m^2 kg s^{-3}
electric charge, quantity (Q), flux (ψ)	coulomb	C	s A
electric potential (V, ϕ), pot. difference (U), emf (E)	volt	V	W/A or J/C = m^2 kg s^{-3} A^{-1}
capacitance (C)	farad	F	C/V = m^{-2} kg^{-1} s^4 A^2
electric resistance (R), impedance (Z)	ohm	Ω	V/A = m^2 kg s^{-3} A^{-2}
electric conductance ($G = 1/R$)	siemens	S	A/V or Ω^{-1} = m^{-2} kg^{-1} s^3 A^2
magnetic flux (Φ)	weber	Wb	V s = m^2 kg s^{-2} A^{-1}
magnetic flux density, induction ($\boldsymbol{B}$)	tesla	T	Wb/m^2 = V s m^{-2} = kg s^{-2} A^{-1}
inductance (L)	henry	H	Wb/A or V s A^{-1} = m^2 kg s^{-2} A^{-2}
Celsius temperature (θ, t)	degree Celsius	°C	°C = K – 273.15

Physical Tables

Special SI-derived Quantities	Unit Name	Symbol	SI-derived and Base Units
luminous flux (F)	lumen	lm	cd sr = $m^2\ m^{-2}$ cd
illuminance (E_v)	lux	lx	lm/m^2 = $m^2\ m^{-4}$ cd = m^{-2} cd
activity, radioactive decay (A)	becquerel	Bq	s^{-1}
absorbed dose, specific energy	gray	Gy	J/kg = $m^2\ s^{-2}$
dose equivalent (personal, organ)	sievert	Sv	J/kg = $m^2\ s^{-2}$
catalytic activity	katal	kat	s^{-1} mol

Other SI-derived Quantities	Unit Name	SI Symbol	SI Base Units
angular velocity (ω)	radian per second	rad/s	s^{-1} [1 Hz = 2π rad s^{-1}]
angular acceleration	radian per second squared	rad/s^2	s^{-2}
moment of force (***M***), torque (***T*** = ***r*** × ***F***)	newton meter	N m	m^2 kg s^{-2}
dynamic viscosity (η, μ)	pascal second	Pa s	N s/m^2 = m^{-1} kg s^{-1}
surface tension (γ, σ)	newton per meter	N/m	kg s^{-2}
specific energy	joule per kilogram	J/kg	$m^2\ s^{-2}$
molar energy	joule per mole	J/mol	m^2 kg s^{-2} mol^{-1}
energy density	joule per cubic meter	J/m^3	m^{-1} kg s^{-2}
heat flux density (I)	watt per square meter	W/m^2	kg s^{-3}
thermal conductivity (λ, k)	watt per meter kelvin	W/(m K)	m kg s^{-3} K^{-1}
heat capacity (C_v , C_p), entropy (S)	joule per kelvin	J/K	m^2 kg s^{-2} K^{-1}
specific heat capacity (c) or entropy	joule per kilogram kelvin	J/(kg K)	$m^2\ s^{-2}\ K^{-1}$
molar entropy, molar heat capacity (C_m)	joule per mole kelvin	J/(mol K)	m^2 kg s^{-2} K^{-1} mol^{-1}
electric field strength (***E***)	volt per meter	V/m	m kg s^{-3} A^{-1}
electric field gradient (q_{ab})	volt per square meter	V/m^2	kg s^{-3} A^{-1}
electric charge density (ρ)	coulomb per cubic meter	C/m^3	m^{-3} s A
electric flux density (***D***)	coulomb per square meter	C/m^2	m^{-2} s A
electric polarization (***P*** = ***D*** − ε_0***E***)	coulomb per square meter	C/m^2	m^{-2} s A
electric dipole moment (μ)	coulomb meter	C m	m s A
electric polarizability (α)		$C^2\ m^2\ J^{-1}$	F m^2 = $kg^{-1}\ s^4\ A^2$
electric quadrupole moment (eQ)	coulomb square meter	C m^2	m^2 s A
electric resistivity ($\rho = E / j$)	ohm meter	Ω m	m^3 kg s^{-3} A^{-2}
electric conductivity ($\kappa = 1 / \rho$)	siemens per meter	S/m	m^{-3} kg^{-1} $s^3\ A^2$
molar conductivity (Λ)	siemens square meter per mole	S m^2/mol	$kg^{-1}\ s^3\ A^2\ mol^{-1}$
permittivity (ε)	farad per meter	F/m	m^{-3} kg^{-1} $s^4\ A^2$
permeability (μ = ***B/H***)	henry per meter	H/m	m kg s^{-2} A^{-2}
exposure (radiation), ion dose	coulomb per kilogram	C/kg	kg^{-1} s A
absorbed dose rate	gray per second	Gy/s	$m^2\ s^{-3}$
rf specific absorption rate (SAR)	watt per kg	W/kg	$m^2\ s^{-3}$
radiant intensity (I)	watt per steradian	W/sr	m^2 kg s^{-3}
radiance (L)	watt per square meter steradian	W/(m^2 sr)	kg s^{-3}
irradiance (E)	watt per square meter	W/m^2	kg s^{-3}
luminous energy (Q_v)	lumen second	lm s	s cd sr
catalytic activity concentration	katal per cubic meter	kat/m^3	m^{-3} s^{-1} mol

Physical Tables

Accepted non-SI units	Unit Name	Symbol	Value in SI units
length	astronomical unit	ua, AU	1 ua = 1.495 978 70 (30) × 10^{11} m
	nautical mile	nmi, NM	1 nautical mile = 1852 m
	Ångström	Å	1 Å = 10^{-10} m = 0.1 nm
area	are	a	1 a = 1 dam^2 = 10^2 m^2
	hectare	ha	1 ha = 1hm^2 = 10^4 m^2
	barn	b	1 b = 100 fm^2 = 10^{-28} m^2
volume	liter	L (l)	1 L = 1 dm^3 = 10^{-3} m^3
concentration	moles per liter (molar, M)	mol/L	1 M = 1 mol/dm^3
time	minute	min	1 min = 60 s
	hour	h	1 h = 60 min = 3600 s
	day	d	1 d = 24 h = 86 400 s
angular measure	degree	°	1° = (π/180) rad = 60'
	minute	'	1' = (1/60)° = (π/10800) rad
	second	''	1'' = (1/60)' = (π/648000) rad
mass	atomic mass unit	u	1 u = 1.660 538 86 (28) × 10^{-27} kg
	metric ton	t	1 t = 1000 kg
velocity	knot = 1 naut. mile/h	kn	1 nmi/h = 0.514444444 m/s
energy	electronvolt	eV	1 eV = 1.602 176 53 (14) × 10^{-19} J
pressure	bar	bar	1 bar = 10^5 Pa = 1000 hPa
nat. log. intensity scale	neper	Np	1 Np = 1 (= 8.6858896 dB)
base-10 log. intensity scale	bel, decibel	B, dB	1 dB = (1n 10)/20 Np

CGS Units	Symbol	SI Value	CGS Units	Symbol	SI Value
erg	erg	1 g cm^2 s^{-2} = 10^{-7} J	dyne	dyn	1 g cm s^{-2} = 10^{-5} N
gal	Gal	1 cm/s^2 = 10^{-2} m/s^2	gauss	G	10^{-4} T = 0.1 mT
maxwell	Mx	10^{-8} Wb	oersted	Oe	(10^3/4π) A/m
phot	ph	10^4 lx	poise	P	1 dyn s /cm^2 = 10^{-1} Pa s
stilb	sb	1 cd/cm^2 = 10^4 cd/m^2	stokes	St	1 cm^2/s = 10^{-4} m^2 s^{-1}

non-SI Units	Symbol	SI Value	non-SI Units	Symbol	SI Value
acceleration	g_n	9.80665 m s^{-2}	atmosphere	atm	101325 Pa
bohr (au)	a_0, b	5.29177 × 10^{-11} m	calorie (therm.)	calth	4.184 J
calorie (intern.)	cal_{IT}	4.1868 J	carat (metric)	kt	200 mg
centipoise	cP	1 mPa s	curie	Ci	3.7 × 10^{10} Bq
dalton	Da, u	1.66053873 × 10^{-27} kg	debye	D	3.33564 × 10^{-30} C m
entropy unit	e.u.	4.184 J K^{-1} mol^{-1}	fermi	f, fm	1 fm = 10^{-15} m
footcandle		10.76391 lx	gamma	γ	1 nT = 10^{-9} T
horsepower	hp	745.6999 W	jansky	Jy	1 Jy = 10^{-26} W m^{-2} Hz^{-1}
lambert		$10^4/\pi$ = 3.183099 cd/m^2	light year	l.y.	9.46073047258 × 10^{15} m
mho		1 siemens	miles/gal. (US)	mpg	235.215/mpg = L/100 km
miles/h	mph	0.44704 m/s	parsec	pc	3.085677581 × 10^{16} m
point (1/72 in)	pt	0.3527778 mm	pound/in^2	psi	6.894757 kPa
quad (10^{15} Btu)		1.055056 × 10^{18} J	rad	rad	1 cGy = 10^{-2} Gy
rem	rem	1 cSv = 10^{-2} Sv	roentgen	R	1 R = 2.58 × 10^{-4} C/kg
svedberg	S, Sv	10^{-13} s	ton (TNT)		4.184 GJ
ton (register)		2.831685 m^3	torr (mm hg)	Torr	1/760 atm = 133.322 3684 Pa
X unit		ca. 1.002 × 10^{-4} nm	year (Gregorian)	a	365.2425 d 31 556 952 s

SI Values of US and Imperial Measures

Linear Measures (1 m = 10^2 cm = 10^3 mm)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (m)**
mil; thou	mil	0.001 in	2.54 E-05
point (font sizes)	pt	1/72 in	3.527778 E-04
pica		12 pt	4.233333 E-03
inch (international)	**in**	**defined**	**0.0254**
inch (US survey)	in	defined: 39.3700 in = 1 m	0.0254000508001016
hand		4 in	0.1016
link (US survey)	li, lnk	33/50 ft	0.201168402336805
foot (int.)	**ft**	**12 in (int)**	**0.3048**
foot (US survey)	ft	defined: 1 ft = 12/39.37 m	0.304800609601219
yard (int.)	**yd**	**3 ft; 36 in (int)**	**0.9144**
yard (US survey)	yd	3 ft; 36 in	0.914401828803658
fathom (US survey)	fm	6 ft	1.82880365760732
rod (US survey)	rd	25 li; 5.5 yd; 16.5 ft	5.02921005842012
chain (US survey)	ch	4 rd; 100 li; 22 yd; 66 ft	20.1168402336805
furlong (US survey)	fur	10 ch; 40 rd; 220 yd; 660 ft	201.168402336805
cable (US survey)		120 fm; 720 ft	219.456438912878
mile (int.)	**mi**	**1760 yd; 5280 ft (int)**	**1609.344**
statute mile (US survey)	mi	25 rd; 80 ch; 5280 ft; 8000 li	1609.347219
nautical mile (int.)	**nmi**	**defined**	**1852**
sea mile (US survey)		6080.20 ft	1853.24866649733
league	lea	3 nautical miles	5556
Area Measures ($1\ m^2 = 10^4\ cm^2 = 10^6\ mm^2$)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (m^2)**
square inch (int.)	sq in, in^2		6.4516 E-04
square foot (int.)	sq ft, ft^2	144 in^2	0.09290304
square yard (int.)	sq yd, yd^2	9 ft^2; 1296 in^2	0.83612736
square rod (US survey)	sq rd, rd^2	30.25 yd^2; 272.25 ft^2	25.2929538117141
acre (international)		4840 yd^2; 43560 ft^2; 0.40468564 ha	4046.8564224
acre (US survey)		10 ch^2; 160 rd^2; 4840 yd^2; 43560 ft^2	4046.87260987425
square mile (int.)	sq mi, mi^2	3097600 yd^2	2.589988110336 E+06
square mile (US survey)	sq mi, mi^2	640 acre	2.58999847031952 E+06
Volume Measures ($1\ L = 1\ dm^3 = 10^{-3}\ m^3$; $1\ mL = 1\ cm^3 = 10^{-6}\ m^3$; $1\ \mu l = 1\ mm^3 = 10^{-9}\ m^3$)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (L, dm^3)**
cubic inch (int.)	cu in, in^3	0.554 fl oz	0.016387064
cubic foot (int.)	cu ft, ft^3	1728 in^3	28.316846592
cubic yard (int.)	cu yd, yd^3	27 ft^3; 46656 in^3	764.554857984
displacement ton		defined as 35 ft^3	991.08963072
register ton		defined as 100 ft^3	2831.6846592
cubic mile (int.)	cu mi, mi^3	5.451776 E9 yd^3	4.168181825 E+12
	Imperial dry and fluid measures (UK, Commonwealth)		
minim	min	1/480 fl oz	5.919388021 E-05
drop	gtt	1/288 fl oz; 5/3 min	9.865646701 E-05
dash		1/384 gi; 1/16 tsp	3.699617513 E-04
pinch		2 dash; 1/192 gi; 1/8 tsp	7.399235026 E-04
scruple	fl s	1/24 fl oz; 20 min	1.183877604 E-03
drachm	fl dr	1/8 fl oz; 60 min	3.551633000 E-03
teaspoon (Canada)	tsp	1/6 fl oz; 80 min	4.735510417 E-03
teaspoon	tsp	1/24 gi; 5/3 fl dr; 100 min	5.919388021 E-03
tablespoon (Canada)	tbsp	1/2 fl oz; 3 tsp; 240 min;	1.420653125 E-02
tablespoon	tbsp	1/8 gi; 5/8 fl oz; 3 tsp; 5 fl dr; 300 min	1.775816406 E-02
ounce (Imp)	**fl oz (Imp)**	**8 fl dr; 480 min**	**0.0284130625**
gill	gi (Imp)	5 fl oz	0.1420653125
cup (Canada)	c (CA)	8 fl oz	0.2273045

Imperial dry and fluid measures (UK, Commonwealth)			
Name	**Symbol**	**Equivalents**	**SI Value (L, dm^3)**
pint	pt (Imp)	4 gill; 20 fl oz	0.56826125
quart	qt (Imp)	2 pt; 40 fl oz	1.1365225
gallon (Imperial)	**gal (Imp)**	**defined as 160 oz av water at 62 °F; 4 qt; 8 pt; 32 gi; 160 fl oz**	**4.54609**
peck	pk	2 gal	9.09218
bucket	bkt	4 gal	18.18436
bushel	bu	8 gal	36.36872
barrel	bl	36 gal	163.65924
		US fluid measures	
minim	min	1/480 fl oz	6.161151992 E-05
drop	gtt	1/360 fl oz; 4/3 min	8.214869323 E-05
dash		1/96 fl oz; 1/16 tsp	3.080575996 E-04
pinch		2 dash; 1/48 fl oz; 1/8 tsp	6.161151992 E-04
dram	fl dr	1/8 fl oz; 60 min	3.696691195 E-03
teaspoon	tsp	1/6 fl oz	4.928921594 E-03
tablespoon	tbsp	1/2 fl oz; 4 fl dr; 0.5 fl oz	1.478676478 E-02
ounce (US)	**fl oz (US)**	**1/128 gal; 8 fl dr; 480 min**	**0.0295735295625**
jigger		1.5 fl oz; 12 fl dr	0.044360294
gill	gi (US)	4 fl oz	0.118294118
cup	c (US)	8 fl oz	0.236588
pint	pt (US)	2 c; 16 fl oz	0.473176473
quart	qt (US)	2 pt; 32 fl oz	0.946353
gallon (US)	**gal (US)**	**defined as 231 in^3; 4 qt; 128 fl oz**	**3.785411784**
barrel	fl bl (US)	defined as 31.5 gal	119.240471196
barrel (oil)	bbl	defined as 42 gal (US)	158.987294928
		US dry measures	
pint	pt	1/64 bu	0.5506104713575
quart	qt	1/32 bu; 2 pt	1.101220942715
board-foot	fbm	defined as 144 in^3	2.359737216
gal	gal	1/8 bu; 4 qt	4.40488377086
peck	pk	1/4 bu; 8 qt	8.80976754172
bushel (dry level)	bu (US lvl)	defined as 2150.42 in^3; 4 pk; 32 qt;	35.23907016688
barrel	bl	105 qt	115.628198985075
seam		8 bu	281.91256133504
cord	cd	128 ft^3	3624.556363776
Mass (1 kg = 10^3 g = 10^6 mg)			
Name	**Symbol**	**Equivalents**	**Exact SI Value (kg)**
avoirdupois	av		
grain	gr	1/7000 lb	6.479891 E-05
dram	dr av	1/256 lb; 7000/256 gr	1.7718451953125 E-03
ounce	oz av	1/16 lb; 16 dr	2.8349523125 E-02
pound	**lb av**	**defined**	**0.45359237**
stone (UK)		14 lb	6.35029318
quarter (UK)		2 stone; 28 lb	12.70058636
hundredweight (short, US)	net cwt	100 lb	45.359237
hundredweight (long, UK)	gross cwt	8 stone; 112 lb	50.80234544
short ton (US)	ton	20 cwt; 2000 lb	907.18474
long ton (UK)	ton	20 cwt (UK); 2240 lb	1016.0469088
troy or apothecary	t, ap		
grain	gr	same mass as in avoirdupois	6.479891 E-05
scruple	s ap	1/24 oz t; 20 gr	1.2959782 E-03
pennyweight	dwt, pwt	1/20 oz t; 24 gr	1.55517384 E-03
dram	dr t	1/8 oz t; 60 gr	3.8879346 E-03
ounce	oz t	1/12 lb t; 20 dwt; 8 dr t; 480 gr	3.11034768 E-02
pound	lb t	12 oz t; 96 dr t; 5760 gr	0.3732417216

Conversion Factors for Important Physical Units

Energy Equivalents

	Joule	Hertz	cm^{-1}	Kelvin	eV
Joule	1	1.5091905 E+33	5.03411762 E+22	7.242964 E+22	6.24150974 E+18
Hertz	6.62606876 E–34	1	3.335640952 E–11	4.7992374 E–11	4.13566727 E–15
cm^{-1}	1.98644544 E–23	2.99792458 E+10	1	1.4387752	1.239841857 E–04
Kelvin	1.3806503 E–23	2.0836644 E+10	0.6950356	1	8.6173432 E–05
eV	1.602176462 E–19	2.417989491 E+14	8.06554477 E+03	1.1604506 E+04	1

based on the Fundamental constants with $E = mc^2 = hc/\lambda = h\nu = kT$ and 1 eV = (e/C) J

Force Units: Si unit = Newton (N), cgs unit = dyne, Weight = mass×g_n

	N	p (pond)	kp	dyne
N	1	101.9716	0.1019716	1.0 E+05
p	0.00980665	1	1.00 E–03	980.665
kp	9.80665	1000	1	980665
dyne	1.0 E–05	1.019716 E–03	1.019716 E–06	1

Energy and Work Units: SI unit = Joule (J), cgs unit: 1 erg = 10^{-7} Joule

	J = N m	kp m	kWh	kcal	BTU	eV
J	1	0.101972	2.777778 E–07	2.390057 E–04	9.478134 E–04	6.241512 E+18
kp m	9.80665	1	2.724069 E–06	2.343846 E–03	9.294874 E–03	6.120832 E+19
kWh	3.600 E+06	3.670978 E+05	1	860.4207	3412.128	2.246944 E+25
kcal	4184	426.6493	1.162222 E–03	1	3.965651	2.611448 E+22
BTU	1055.06	1.075862 E+02	2.930722 E–01	2.521654 E–01	1	6.585169 E+21
eV	1.602176 E–19	1.633765 E–20	4.450489 E–26	3.829293 E–23	1.518564 E–22	1

Power Units: SI unit = Watt (W)

	W = J s^{-1}	kW	kpm/s	PS	cal/s	kcal/h
W	1	1.0 E–03	0.1019716	1.341022 E–03	0.2390057	0.8604207
kW	1.0 E+03	1	101.9716	1.341022	239.0057	860.4207
kpm/s	9.80665	9.80665 E–03	1	1.315093 E–02	2.343846	8.437844
PS	745.7	0.7457	76.04024	1	178.2266	641.6157
cal/s	4.184	4.184 E–03	0.4266493	5.610835 E–03	1	3.6
kcal/h	1.162222	1.162222 E–03	0.1185137	1.558565 E–03	0.2777778	1

Pressure Units: SI unit = Pascal

	Pa = N/m^2	kp/m^2	atm	bar	Torr = mmHg	at = kp/cm^2
Pa = N/m^2	1	0.1019716	9.86923 E–06	1.0 E–05	7.500617 E–03	1.019716 E–05
kp/m^2	9.80665	1	9.67841 E–05	9.80665 E–05	7.355592 E–02	1.0 E–04
atm	1.01325 E+05	1.033227 E+04	1	1.01325	760	1.033227
bar	1.0 E+05	1.019716 E+04	0.9869233	1	750.0617	1.019716
Torr	133.3224	13.59510	1.315789 E–03	1.333224 E–03	1	1.359510 E–03
at = kp/cm^2	9.80665 E+04	1.0 E+04	0.9678411	9.800665 E–01	735.5592	1

Time Units: SI unit = second

	s	min	h	d	week	year
s	1	1.666667 E–02	2.777778 E–04	1.157407 E–05	1.653439 E–06	3.168874 E–08
min	60	1	1.666667 E–02	6.944444 E–04	9.920635 E–05	1.901324 E–06
h	3600	60	1	4.166667 E–02	5.952381 E–03	1.140795 E–04
d	86400	1440	24	1	1.428571 E–01	2.737907 E–03
week	604800	10080	168	7	1	1.916535 E–02
year	31556952	525949.2	8765.82	365.2425	52.1775	1

Temperature Conversion: SI unit = Kelvin

	Kelvin (K)	Centigrade (°C)	Fahrenheit (°F)	Rankine (°R)
K	1	$T_C = T_K - 273.15$	$T_F = (9/5)T_K - 459.67$	$T_R = (9/5)T_K$
°C	$T_K = T_C + 273.15$	1	$T_F = (9/5)T_C + 32$	$T_R = (9/5)(T_C + 273.15)$
°F	$T_K = (5/9)(T_F + 459.67)$	$T_C = (5/9)(T_F - 32)$	1	$T_R = T_F + 459.67$
°R	$T_K = (9/5)T_R$	$T_C = (5/9)T_R - 273.15$	$T_F = T_R - 459.67$	1

Physical Tables

Colour, Wave Length, Frequency, Wave Number and Energy of Light

Colour	λ [nm]	ν [Hz]	ν [cm^{-1}]	E [eV]	E [kJ mol^{-1}]
Infrared	1000	$3.00 \cdot 10^{14}$	$1.00 \cdot 10^{4}$	1.24	120
Red	700	$4.28 \cdot 10^{14}$	$1.43 \cdot 10^{4}$	1.77	171
Orange	620	$4.84 \cdot 10^{14}$	$1.61 \cdot 10^{4}$	2.00	193
Yellow	580	$5.17 \cdot 10^{14}$	$1.72 \cdot 10^{4}$	2.14	206
Green	530	$5.66 \cdot 10^{14}$	$1.89 \cdot 10^{4}$	2.34	226
Blue	470	$6.38 \cdot 10^{14}$	$2.13 \cdot 10^{4}$	2.64	254
Violet	420	$7.14 \cdot 10^{14}$	$2.38 \cdot 10^{4}$	2.95	285
Near Ultraviolet	300	$1.00 \cdot 10^{15}$	$3.33 \cdot 10^{4}$	4.15	400
Far Ultraviolet	200	$1.50 \cdot 10^{15}$	$5.00 \cdot 10^{4}$	6.20	598

Density of Water (H_2O)

t [°C]	ρ [kg/dm^3]	t [°C]	ρ [kg/dm^3]	t [°C]	ρ [kg/dm^3]
0	0.999841	11	0.999606	22	0.997772
1	0.999900	12	0.999498	23	0.997540
2	0.999941	13	0.999377	24	0.997299
3	0.999965	14	0.999244	25	0.997047
4	0.999973	15	0.999099	26	0.996785
5	0.999965	16	0.998943	27	0.996515
6	0.999941	17	0.998775	28	0.996235
7	0.999902	18	0.998596	29	0.995946
8	0.999849	19	0.998406	30	0.995649
9	0.999782	20	0.998205		
10	0.999701	21	0.997994		

Viscosity of Water, η in mPa · s (cP)

t [°C]	η	t [°C]	η	t [°C]	η	t [°C]	η
0	1.7865	**20**	1.0019	**50**	0.5477	**90**	0.3155
5	1.5138	**25**	0.8909	**60**	0.4674	**100**	0.2829
10	1.3037	**30**	0.7982	**70**	0.4048	**125**	0.2200
15	1.1369	**40**	0.6540	**80**	0.3554	**150**	0.1830

Physical Tables

Viscosities of Various Liquids, η in mPa · s (cP)

Liquid	0°C	10°C	20°C	30°C	40°C	50°C	60°C	70°C	100°C
Acetic acid	–	–	1.219	1.037	0.902	0.794	0.703	0.629	0.464
Acetone	0.397	0.358	0.324	0.295	0.272	0.251	–	–	–
Aniline	–	6.53	4.39	3.18	2.40	1.91	1.56	1.29	0.76
Benzene	–	0.757	0.647	0.560	0.491	0.435	0.389	0.350	–
Bromobenzene	1.556	1.325	1.148	1.007	0.889	0.792	0.718	0.654	0.514
Carbon disulfide	0.436	0.404	0.375	0.351	0.329	–	–	–	–
Carbon dioxide (liq.)	0.099	0.085	0.071	0.053	–	–	–	–	–
Carbon tetrachloride	1.348	1.135	0.972	0.845	0.744	0.660	0.591	0.533	0.400
Chloroform	0.704	0.631	0.569	0.518	0.473	0.434	0.399	–	–
Diethyl ether	0.294	0.267	0.242	0.219	0.199	0.183	0.168	0.154	0.119
Ethanol	1.767	1.447	1.197	1.000	0.830	0.700	0.594	0.502	–
Ethyl acetate	0.581	0.510	0.454	0.406	0.366	0.332	0.304	0.278	–
Ethyl formate	0.508	0.453	0.408	0.368	0.335	0.307	–	–	–
Formic acid	–	2.241	1.779	1.456	1.215	1.033	0.889	0.778	0.547
Mercury	1.681	1.661	1.552	1.499	1.450	1.407	1.367	1.327	1.232
Methanol	0.814	0.688	0.594	0.518	0.456	0.402	0.356	–	–
***n*-Octane**	0.710	0.618	0.545	0.485	0.436	0.494	0.358	0.326	0.255
Oil, castor	–	2420	986	451	231	125	74	43	16.9
Oil, olive	–	138	84	52	36	24.5	17	12.4	–
***n*-Pentane**	0.278	0.254	0.234	0.215	0.198	0.184	0.172	0.161	0.130
Sulfuric acid	56	49	27	20	14.5	11.0	8.2	6.2	–
Toluene	0.771	0.668	0.585	0.519	0.464	0.418	0.379	0.345	0.268

Self-Diffusion Coefficients *D* of Various Liquids at 25°C

Liquid	D [$10^{-9}m^2s^{-1}$]	Liquid	D [$10^{-9}m^2s^{-1}$]	Liquid	D [$10^{-9}m^2s^{-1}$]
Water (H_2O)	2.299	Acetonitrile	4.37	Cyclopentane	3.09
Water (D_2O)	1.872	Pyridine	1.54	Cyclooctane	0.55
Methanol (CH_3OH)	2.415	Nitromethane	2.39	*n*-Pentane	5.72
Methanol (CH_3OD)	2.30	Tetrahydrofuran	2.84	*n*-Hexane	4.26
Methanol (CD_3OH)	2.21	Benzene	2.21	*n*-Heptane	3.12
Methanol (CD_3OD)	2.11	Fluorobenzene	2.39	*n*-Octane	2.35_5
Ethanol	1.08	Hexafluorobenzene	1.46	*n*-Nonane	1.77
t-Butanol-d_1	0.28	Toluene	2.27	*N*-Decane	1.37
Formamide	0.55	Carbon disulfide	4.32	*n*-Undecane	1.07_6
N,N-Dimethylformamide	1.63	Carbon Tetrachloride	1.30	*n*-Dodecane	0.81
N,N-Dimethylacetamide	1.35	Chloroform	2.35	*n*-Tridecane	0.70
Dimethyl sulfoxide	0.73	Acetic acid	1.08	*n*-Tetradecane	0.52
Dioxane	1.09	Formic acid	1.08	Pentan-1-ol	0.29
Acetone	4.57	Cyclohexane	1.42	Octan-1-ol	0.14

Table by courtesy of Dr. M. Holz (Institute of Phys. Chem., University of Karlsruhe, FRG) and Prof. A Sacco (Dept. Chem., University of Bari, Italy).

Temperature Dependence of the Self-Diffusion Coefficient *D* of Water (H_2O)

t [°C]	D [$10^{-9}m^2s^{-1}$]	t [°C]	D [$10^{-9}m^2s^{-1}$]	t [°C]	D [$10^{-9}m^2s^{-1}$]	t [°C]	D [$10^{-9}m^2s^{-1}$]
-5	0.913	20	2.023	50	3.956	80	6.557
0	1.099	25	2.299	55	4.344	85	7.056
2.5	1.199	30	2.594	60	4.748	90	7.574
5	1.303	35	2.907	65	5.172	95	8.111
10	1.525	40	3.238	70	5.615	100	8.667
15	1.765	45	3.588	75	6.078		

Table by courtesy of Dr. M. Holz, Institute of Phys. Chem., University of Karlsruhe, FRG.

International Dialing Codes / World Time Zones

Time Zones are listed as increment in hour:min relative to UTC / GMT for ST = standard time; DST = Daylight Savings (Summer) Time (where used). Provences or Cities are listed for countries with more than one time zone.

NB: DST runs approximately from March to October in the northern hemisphere and October to March in the southern hemisphere; exact period depends on country and may change from year to year. (data adapted by W.E. Hull from www.happyzebra.com and www.worldtimezone.com)

Country (Code) - Provinces / Cities	ST	DST
Afghanistan (+93)	+4:30	
Albania (+355)	+1	+2
Algeria (+213)	+1	
Angola (+244)	+1	
Argentina (+54) DST only in Buenos Aires and some provinces in the northeast	–3	–2
Armenia (+374)	+4	+5
Australia (+61) - W. Austr. (Perth)	+8	
Australia (+61) - N. Terr. (Darwin),	+9:30	
Australia (+61) - Queensland (Brisbane)	+10	
Australia (+61) - Cap. Terr. (Canberra), N.S.W. (Sydney), Victoria (Melbourne), S. Austr. (Adelaide), Tasmania (Hobart)	+10	+11
Austria (+43)	+1	+2
Azerbaijan (+994)	+4	+5
Bahamas (+1)	–5	–4
Bahrain (+973)	+3	
Bangladesh (+880)	+6	+7
Barbados (+1)	–4	
Belarus (+375)	+2	+3
Belgium (+32)	+1	+2
Belize (+501)	–6	
Benin (+229)	+1	
Bermuda (UK)	–4	–3
Bhutan (+975)	+6	
Bolivia (+591)	–4	
Bosnia-Herzegovina (+387)	+1	+2
Botswana (+267)	+2	
Brazil (+55) / Rio Branco	–5	
Brazil (+55) / Manaus	–4	
Brazil (+55) / Salvador, Recife	–3	
Brazil (+55) / Brasilia, Rio de Janeiro, Porto Alegre, Sao Paulo	–3	–2
Brazil (+55) / Fernando de Noronha	–2	
Brunei (+673)	+8	
Bulgaria (+359)	+2	+3
Burkina Faso (+226)	0	
Burundi (+257)	+2	
Cambodia (+855)	+7	
Cameroon (+237)	+1	
Canada (+1) - Newfoundland & Labrador	–3:30	–2:30
Canada (+1) - Pr. Edward Island, Nova Scotia, New Brunswick	–4	–3
Canada (+1) - Ontario (Toronto, Ottawa), Quebec (Montreal, Quebec)	–5	–4
Canada (+1) - Manitoba (Winnipeg)	–6	–5
Canada (+1) - Alberta (Edmonton, Calgary), NW Territories	–7	–6
Canada (+1) - Saskatchewan	–7	
Canada (+1) - British Columbia (Vancouver), Yukon Terr.	–8	–7
Canary Islands (Spain)	0	+1
Central African Republic (+236)	+1	
Chad (+235)	+1	
Chile (+56)	–4	–3
China (+86)	+8	
Colombia (+57)	–5	
Congo, Repub. (+242) / Kinshasa	+1	

Country (Code) - Provinces / Cities	ST	DST
Congo, Dem. Repub. (+243) / Lubumbashi	+2	
Costa Rica (+506)	–6	
Cote dĺvoire (+225)	0	
Croatia (+385)	+1	+2
Cuba (+53)	–5	–4
Cyprus (+357)	+2	+3
Czech Republic (+420)	+1	+2
Denmark (+45)	+1	+2
Djibouti (+253)	+3	
Dominican Republic (+1)	–4	
Ecuador (+593)	–5	
Egypt (+20)	+2	+3
El Salvador (+503)	–6	
Eritrea (+291)	+3	
Estonia (+372)	+2	+3
Ethiopia (+251)	+3	
Fiji (+679)	+12	
Finland (+358)	+2	+3
France (+33)	+1	+2
French Guiana	–3	
Gabon (+241)	+1	
Galapagos Islands (Ecuador)	–6	
Gambia (+220)	0	
Gaza (+970)	+2	+3
Georgia (+995)	+4	
Germany (+49)	+1	+2
Ghana (+233)	0	
Gibraltar (UK)	+1	+2
Greece (+30)	+2	+3
Guatemala (+502)	–6	
Guadeloupe (France)	–4	
Guinea (+224)	0	
Guyana (+592)	–4	
Haiti (+509)	–5	
Honduras (+504)	–6	
Hungary (+36)	+1	+2
Iceland (+354)	0	
India (+91)	+5:30	
Indonesia (+62) - Papua	+9	
Indonesia (+62) - Bali, Kalimantan, Lombok, West Timor	+8	
Indonesia (+62) - Java, Sumatra	+7	
Iran (+98)	+3:30	+4:30
Iraq (+964)	+3	
Ireland (+353)	0	+1
Israel (+972)	+2	+3
Italy (+39)	+1	+2
Jamaica (+1)	–5	
Japan (+81)	+9	
Jordan (+962)	+2	+3
Kazakhstan (+7) / Almaty, Astana	+6	
Kazakhstan (+7) / Aqtau, Aqtobe	+5	
Kenya (+254)	+3	
Kosovo (+381)	+1	+2
Kuwait (+965)	+3	

International Dialing Codes / World Time Zones

Country (Code) - Provinces / Cities	ST	DST
Kyrgyzstan (+996)	+6	
Laos (+856)	+7	
Latvia (+371)	+2	+3
Lebanon (+961)	+2	+3
Lesotho (+266)	+2	
Liberia (+231)	0	
Libya (+218)	+2	
Liechtenstein (+423)	+1	+2
Lithuania (+370)	+2	+3
Luxembourg (+352)	+1	+2
Macedonia (+389)	+1	+2
Madagascar (+261)	+3	
Malawi (+265)	+2	
Malaysia (+60)	+8	
Maldives (+960)	+5	
Mali (+223)	0	
Malta (+356)	+1	+2
Martinique (France)	–4	
Mauritania (+222)	0	
Mauritius (+230)	+4	
Mexico (+52) - Aguascalientes, Fed. District (Mexico City), Guanajuato, Guerrero, Jalisco, Nuevo Leon, Quintana Roo, San Luis Potosi, Veracruz, Yucatan	–6	–5
Mexico (+52) - Chihuahua, Sinaloa	–7	–6
Mexico (+52) - Sonorro	–7	
Mexico (+52) - Baja California (Tijuana)	–8	–7
Moldova (+373)	+2	+3
Monaco (+377)	+1	+2
Mongolia (+976) / Choibalsan, Ulaanbaatar	+8	
Mongolia (+976) / Hovd	+7	
Montenegro (+382)	+1	+2
Morocco (+212)	0	+1
Mozambique (+258)	+2	
Myanmar (+95)	+6:30	
Namibia (+264)	+1	+2
Nepal (+977)	+5:45	
Netherlands (+31)	+1	+2
New Zealand (+64)	+12	+13
Nicaragua (+505)	–6	
Niger (+227)	+1	
Nigeria (+234)	+1	
North Korea (+850)	+9	
Norway (+47)	+1	+2
Oman (+968)	+4	
Pakistan (+92)	+5	+6
Panama (+507)	–5	
Papua New Guinea (+675)	+10	
Paraguay (+595)	–4	–3
Peru (+51)	–5	
Philippines (+63)	+8	
Poland (+48)	+1	+2
Portugal (+351)	0	+1
Puerto Rico (+1)	–4	
Qatar (+974)	+3	
Reunion (+262)	+4	
Romania (+40)	+2	+3
Russia (+7) / Kaliningrad	+2	+3
Russia (+7) / Kazan, Moscow, Murmansk, Novgorod, St. Petersburg	+3	+4
Russia (+7) / Samara	+4	+5
Russia (+7) / Chelyabinsk, Novosibirsk, Perm, Ufa, Yekaterinburg	+5	+6

Country (Code) - Provinces / Cities	ST	DST
Russia (+7) / Omsk	+6	+7
Russia (+7) / Krasnoyarsk	+7	+8
Russia (+7) / Irkutsk	+8	+9
Russia (+7) / Yakutsk	+9	+10
Russia (+7) / Vladivostok, Yuzhno-Sakhalinsk	+10	+11
Russia (+7) / Magadan	+11	+12
Russia (+7) / Anadyr, Kamchatka	+12	+13
Rwanda (+250)	+2	
Saudi Arabia (+966)	+3	
Senegal (+221)	0	
Serbia (+381)	+1	+2
Seychelles (+248)	+4	
Sierra Leone (+232)	0	
Singapore (+65)	+8	
Slovakia (+421)	+1	+2
Slovenia (+386)	+1	+2
Somalia (+252)	+3	
South Africa (+27)	+2	
South Korea (+82)	+9	
Spain (+34)	+1	+2
Sri Lanka (+94)	+5:30	
Sudan (+249)	+3	
Suriname (+597)	–3	
Swaziland (+268)	+2	
Sweden (+46)	+1	+2
Switzerland (+41)	+1	+2
Syria (+963)	+2	+3
Tahiti (France)	–10	
Taiwan (+886)	+8	
Tajikistan (+992)	+5	
Tanzania (+255)	+3	
Thailand (+66)	+7	
Timor-Leste (+670)	+9	
Togo (+228)	0	
Trinidad & Tobago (+1)	–4	
Tunisia (+216)	+1	
Turkey (+90)	+2	+3
Turkmenistan (+993)	+5	
UAE - Abu Dhabi, Dubai (+971)	+4	
Uganda (+256)	+3	
Ukraine (+380)	+2	+3
United Kingdom (+44) - England, Scotland, Wales, N. Ireland	0	+1
Uruguay (+598)	–3	–2
USA (+1) - Eastern Zone (New York, Boston, Miami, Philadelphia...)	–5	–4
USA (+1) - Central Zone (Chicago, Wichita, New Orleans, Pensicola)	–6	–5
USA (+1) - Mountain Zone (Helena, Denver, Santa Fe)	–7	–6
USA (+1) - Arizona	–7	
USA (+1) - Pacific Zone (Las Vegas, San Francisco, Los Angeles)	–8	–7
USA (+1) - Alaska (Anchorage)	–9	–8
USA (+1) - Hawaii (Honolulu)	–11	
Uzbekistan (+998)	+5	
Vatican City (+39)	+1	+2
Venezuela (+58)	–4:30	
Vietnam (+84)	+7	
Yemen (+967)	+3	
Zambia (+260)	+2	
Zimbabwe (+263)	+2	