^{1}H NMR Chemical Shift Laboratory Data Guide

Compounds	$CDCl_3$	$(CD_3)_2SO$	C_5D_5N or C_5H_5N	C_6D_6 or C_6H_6	D_2O
Acetic acid	2.13	1.95	2.13	1.63	2.16
Acetone	2.17	2.12	2.00	1.62	2.22
Acetonitrile	1.98	2.09	1.85	0.67	2.05
Benzene	7.37	7.40	7.33	7.30	7.44
Bromoform	6.85	7.75	7.86	5.89	Insoluble
n-Butanol	3.67 (t)	3.41 (t)	3.80 (t)	3.38 (t)	3.60 (t)
	0.94 (t)	0.89 (t)	0.89 (t)	0.83 (t)	0.89 (t)
t-Butanol	1.28	1.14	1.37	1.06	1.23
Chloroform	7.27	8.35	8.41	6.41	Insoluble
Cyclohexane	1.43	1.42	1.38	1.40	Insoluble
1,2-Dibromoethane	3.63	3.84	3.70	2.88	3.79
Dichloroacetic acid	5.98	6.68	6.72	5.43	6.21
1,2-Dichloroethane	3.73	3.93	3.78	2.99	3.92
Dichloromethane	5.30	5.79	5.62	4.46	Insoluble
Diethyl ether	3.48 (q)	3.42 (q)	3.38 (q)	3.27 (q)	3.56 (q)
	1.20 (t)	1.13 (t)	1.12 (t)	1.10 (t)	1.17 (t)
N,N-Dimethylformamide-d_7	8.01	7.98	2.72	2.40	7.91
	2.95	2.92	2.66	1.98	3.00
	2.88	2.76			2.86
Dioxane	3.70	3.61	3.61	3.38	3.75
Ethanol	3.72 (q)	3.49 (q)	3.86 (q)	3.39 (q)	3.46 (q)
	1.24 (t)	1.09 (t)	1.29 (t)	0.97 (t)	1.16 (t)
Ethyl acetate	4.12 (q)	4.08 (q)	4.06 (q)	3.91 (q)	4.14 (q)
	2.04	2.02	1.94	1.68	2.08
	1.25 (t)	1.21 (t)	1.10(t)	0.94(t)	1.23 (t)
Ethyl formate	8.04	8.23	8.22	7.60	8.16
	4.22 (q)	4.17 (q)	4.14 (q)	3.83 (q)	4.28 (q)
	1.29 (t)	1.24 (t)	1.10 (t)	0.85 (t)	1.29 (t)
Formic acid	8.02	8.18	8.54	7.24	8.22
Methanol	3.48	3.20	3.57	3.09	3.35
Methyl acetate	3.67	3.61	3.55	3.28	3.68
	2.05	2.02	1.92	1.63	2.09
Methyl iodide	2.16	2.21	Reactive	1.47	Insoluble
Methyl sulfoxide	2.62	2.52	2.49	1.91	2.70
Nitromethane	4.32	4.44	4.39	3.09	4.41
1-Propanol	3.60 (t)	1.45 (m)	3.75 (t)	3.76 (t)	3.61 (t)
	1.60 (m)	0.87 (t)	1.70 (m)	1.40 (m)	1.57 (m)
	0.93 (t)		0.97 (t)	0.80 (t)	0.89 (t)
2-Propanol	4.03 (m)	1.06 (d)	4.16 (m)	3.76 (m)	1.18 (d)
	1.20 (d)		1.29 (d)	1.01 (d)	
Propionic acid	2.42 (q)	2.26 (q)	2.46 (q)	2.02 (q)	2.47 (q)
	1.18 (t)	1.03 (t)	1.20 (t)	0.89 (t)	1.10 (t)
Pyridine	8.60 (m)	8.61 (m)	8.71 (m)	8.50 (m)	8.50 (m)
	7.69 (m)	7.83 (m)	7.58 (m)	7.05 (m)	7.90 (m)
	7.28 (m)	7.40 (m)	7.21 (m)	6.70 (m)	7.46 (m)
1,1,2,2-Tetrachloroethane	5.96	6.92	6.90	4.96	Insoluble
Tetrahydrofuran	3.74 (m)	3.63 (m)	3.67 (m)	3.01 (m)	3.75 (m)
	1.85 (m)	1.78 (m)	1.64 (m)	0.87 (m)	1.88 (m)
Toluene	7.19	7.22	7.22	7.10	Insoluble
	2.34	2.32	2.22	2.13	
1,1,1-Trichloroethane	1.72	2.80	2.61	1.58	Insoluble
Trimethylphosphate	3.80 (d)	3.72 (d)	3.71 (d)	3.37 (d)	3.82 (d)

NMR Solvents Reference Data

Name & Cat. No.	CAS. No.	Mol. Wt.	Density at 25 °C	mp (°C)[a]	bp (°C)[a]	δ_H(Mult)[b]	J_{HD}	δ_C(Mult)[b]	J_{CD} (J_{CF})
Acetic acid-d_4 (151785)	1186-52-3	64.08	1.119	15-16	115.5	11.53 (1)		178.4 (br)	
						2.03 (5)	2	20.0 (7)	20
Acetone-d_6 (151793)	666-52-4	64.12	0.872	-93.8	55.5			206.0 (13)	0.9
						2.04 (5)	2.2	29.8 (7)	20
Acetonitrile-d_3 (151807)	2206-26-0	44.07	0.844	-48	80.7			118.2 (br)	
						1.93 (5)	2.5	1.3 (7)	21
Benzene-d_6 (151815)	1076-43-3	84.15	0.950	6.8	79.1	7.15 (br)		128.0 (3)	24
Chloroform-d (151823)	865-49-6	120.38	1.500	-64	60.9	7.24 (1)		77.0 (3)	32
Cyclohexane-d_{12} (151866)	1735-17-7	96.23	0.893	4-7	80.7	1.38 (br)		26.4 (5)	19
Deuterium oxide (151882)	7789-20-0	20.03	1.107	3.8	101.4	4.84 (DSS)			
						4.81 (TSP)			
Dichloromethane-d_2 (444324)	1665-00-5	86.94	1.362	-97	40	5.32 (3)	1	53.8 (5)	27
N,N-Dimethylformamide-d_7 (189979)	4472-41-7	80.14	1.030	-61	153	8.01 (br)		162.7 (3)	30
						2.91 (5)	2	35.2 (7)	21
						2.74 (5)	2	30.1 (7)	21
Dimethyl sulfoxide-d_6 (151874)	2206-27-1	84.17	1.190	16-19	189	2.49 (5)	1.7	39.5 (7)	21
1,4-Dioxane-d_8 (186406)	17647-74-4	96.15	1.129	10-12	99	3.53 (m)		66.5 (5)	22
Ethanol-d_6 (186414)	1516-08-1	52.11	0.892	-114	78	5.19 (1)			
						3.55 (br)		56.8 (5)	22
						1.11 (m)		17.2 (7)	19
Methanol-d_4 (151947)	811-98-3	36.07	0.888	-98	65.4	4.89 (1)		49.0 (7)	21.4
						3.30 (5)	1.7		
2-Propanol-d_8 (175897)	22739-76-0	68.14	0.890	-89.5	82	5.12 (1)			
						3.89 (br)		62.9 (3)	21.5
Pyridine-d_5 (532975)	7291-22-7	84.13	1.050	-42	114.4	8.71 (br)		149.9 (3)	27.5
						7.55 (br)		135.5 (3)	24.5
						7.19 (br)		123.5 (3)	25
Tetrahydrofuran-d_8 (184314)	1693-74-9	80.16	0.985	-106	65-66	3.58 (br)		67.4 (5)	22
						1.73 (br)		25.3 (br)	20.5
Toluene-d_8 (434388)	2037-26-5	100.19	0.943	-93	110			137.5 (1)	
						7.09 (m)		128.9 (3)	23
						7.00 (br)		128.0 (3)	24
						6.98 (m)		125.2 (3)	24
						2.09 (5)	2.3	20.4 (7)	19
Trifluoroacetic acid-d (152005)	599-00-8	115.03	1.493	-15.4	75	11.50 (1)		164.2 (4)	(44)
								116.6 (4)	(283)
2,2,2-Trifluoroethanol-d_3 (396532)	77253-67-9	103.06	1.415	-44	77-80	5.02 (1)		126.3 (4)	(277)
						3.88 (4 x 3)	2 (9)	61.5 (4 x 5)	22 (36)

[a]Melting and boiling points (in °C) are those of the corresponding natural abundance compound (except for D_2O) and are intended only to indicate the useful liquid range of the materials.
[b]The multiplicity "br" indicates a broad peak without resolvable fine structure, while "m" denotes a broad peak with fine structure.

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