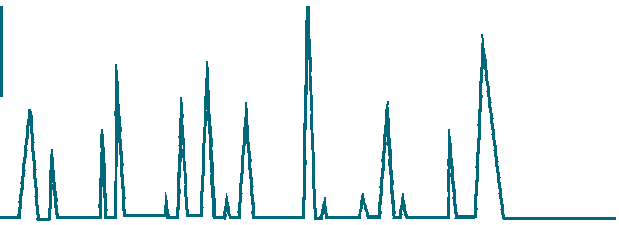
NMR Solvent Data Chart

Cambridge Isotope Labs



SOLVENT	^{1}H Chemical Shift (ppm from TMS) (multiplicity)	JHD (Hz)	Carbon-13 Chemical Shift (ppm from TMS) (multiplicity)	JCD (Hz)	^{1}H Chemical Shift of HOD (ppm from TMS)	Density at 20°C	Melting point (°C)	Boiling point (°C)	Dielectric Constant	Molecular Weight
Acetic Acid-d 4	11.65 (1) 2.04 (5)	2.2	178.99 (1) 20.0 (7)	2.0	11.5	1.12	16	115.5	6.1	64.08
Acetone-d 6	2.05 (5)	2.2	206.68 (1) 29.92 (7)	0.9 19.4	2.8	0.87	-94	57	20.7	64.12
Acetonitrile-d 3	1.94 (5)	2.5	118.69 (1) 1.39 (7)	21	2.1	0.84	-45	82	37.5	44.07
Benzene-d 6	7.16 (1)		128.39 (3)	24.3	0.4	0.95	5	80	2.3	84.15
Chloroform-d	7.24 (1)		77.23 (3)	32.0	1.5	1.50	-64	62	4.8	120.38
Cyclohexane-d 12	1.38 (1)		26.43 (5)	19	0.8	0.89	6	81	2.0	96.24
Deuterium Oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8	1.11	3.8	101.4	78.5	20.03
N, N-Dimethyl -formamide-d 7	8.03 (1) 2.92 (5) 2.75 (5)	 1.9 1.9	163.15 (3) 34.89 (7) 29.76 (7)	29.4 21.0 21.1	3.5	1.04	-61	153	36.7	80.14
Dimethyl Sulfoxide-d 6	2.50 (5)	1.9	39.51 (7)	21.0	3.3	1.18	18	189	46.7	84.17
1,4-Dioxane-d 8	3.53 (m)		66.66 (5)	21.9	2.4	1.13	12	101	2.2	96.16
Ethanol-d 6	5.29 (1) 3.56 (1) 1.11 (m)		 56.96 (5) 17.31 (7)	 22 19	5.3	0.89	<-130	79	24.5	52.11
Methanol-d 4	4.87 (1) 3.31 (5)	 1.7	 49.15 (7)	 21.4	4.9	0.89	-98	65	32.7	36.07
Methylene Chloride-d 2	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	40		86.95
Pyridine-d 5	8.74 (1) 7.58 (1) 7.22 (1)		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 3	5	1.05	-42	116	12.4	84.13
Tetrahydrofuran-d 8	3.58 (1) 1.73 (1)		67.57 (5) 25.37 (5)	22.2 20.2	2.4-2.5	0.99	-109	66	7.6	80.16
Toluene-d 8	 7.09 (m) 7.00 (1) 6.98 (5) 2.09 (5)	 2.3	137.86 (1) 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	 23 24 24 19	0.4	0.94	-95	111	2.4	100.19
Trifluoroacetic Acid-d	11.50 (1)		164.2 (4) 116.6 (4)		11.5	1.50	-15	72		115.03
Trifluoroethanol-d 3	5.02 (1) 3.88 (4x3)	 2(9)	126.3 (4) 61.5 (4X5)	 22	5	1.41	-44	75		103.06

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

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

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

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