NMR SOLVENT DATA CHART

Cambridge Isotope Laboratories, Inc.
www.isotope.com

NMR SOLVENTS

NMR Solvent Data Chart

More Solvents, More Sizes, More Solutions

	^{1}H Chemical Shift (ppm from TMS) (multiplicity) ●	JCD(Hz)	^{13}C 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)	20	11.5	1.12	16.7	118	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	56.5	20.7	64.12
Acetonitrile-d_3	1.94 (5)	2.5	118.69 (1) 1.39 (7)	21	2.1 *	0.84	-45	81.6	37.5	44.07
Benzene-d_6	7.16 (1)		128.39 (3)	24.3	0.4	0.95	5.5	80.1	2.3	84.15
Chloroform-d	7.24 (1)		77.23 (3)	32.0	1.5 *	1.50	-63.5	61-62	4.8	120.38
Cyclohexane-d_{12}	1.38 (1)		26.43 (5)	19	0.8	0.89	6.47	80.7	2.0	96.24
Deuterium Oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8	1.11	3.81	101.42	78.5	20.03
N, N-Dimethyl-formamide-d_7	8.03 (1)		163.15 (3)	29.4	3.5	1.03	-61	153	36.7	80.14
	2.92 (5)	1.9	34.89 (7)	21.0						
	2.75 (5)	1.9	29.76 (7)	21.1						
Dimethyl Sulfoxide-d_6	2.50 (5)	1.9	39.51 (7)	21.0	3.3 *	1.19	18.45	189	46.7	84.17
1,4-Dioxane-d_8	3.53 (m)		66.66 (5)	21.9	2.4	1.13	11.8	101.1	2.2	96.16
Ethanol-d_6	5.19 (1)				5.3	0.89	-114.1	78.5	24.5	52.11
	3.56 (1)		56.96 (5)	22						
	1.11 (m)		17.31 (7)	19						
Methanol-d_4	4.78 (1)				4.9	0.89	-97.8	64.7	32.7	36.07
	3.31 (5)	1.7	49.15 (7)	21.4						
Methylene Chloride-d_2	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	39.75	8.9	86.95
Pyridine-d_5	8.74 (1)		150.35 (3)	27.5	5	1.05	-42	115-116	12.4	84.13
	7.58 (1)		135.91 (3)	24.5						
	7.22 (1)		123.87 (3)	25						
1,1,2,2-Tetrachloroethane-d_2	6.0		73.78 (3)			1.62	-44	147	8.20	169.86
Tetrahydrofuran-d_8	3.58 (1)		67.57 (5)	22.2	2.4-2.5	0.99	-108.5	66	7.6	80.16
	1.73 (1)		25.37 (5)	20.2						
Toluene-d_8			137.86 (1)		0.4	0.94	-95	110.6	2.4	100.19
	7.09 (m)		129.24 (3)	23						
	7.00 (1)		128.33 (3)	24						
	6.98 (5)		125.49 (3)	24						
	2.09 (5)	2.3	20.4 (7)	19						
Trifluoroacetic Acid-d	11.50 (1)		164.2 (4)		11.5	1.41	-15.4	72.4		115.03
			116.6 (4)							
Trifluoroethanol-d_3	5.02 (1)		126.3 (4)		5	1.41	-43.3	75		103.06
	3.88 (4x3)	2(9)	61.5 (4x5)	22						

S Budavari, M.J. O'Neil, A. Smith, P.E. Heckelman, **The *Merck Index*, an Encyclopedia of Chemicals, Drugs, and Biologicals - Eleventh Edition**, Merck Co., Inc. Rahway, NJ, 1989.

● The ^{1}H spectra of the residual protons and ^{13}C spectra were obtained on a Varian Gemini 200 spectrometer at 295°K. The NMR solvents used to acquire these 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 chemical shifts can be dependent on solvent, 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. Information gathered from the Merck Index -Eleventh Edition.

* HOD Peaks - NMR spectra of "neat" deuterated solvent always exhibit a peak due to H_20 in addition to the residual solvent peak. When the exchange rate between H_20 and HDO is slow on the NMR timescale the water peak appears as two peaks, a singlet corresponding to H_20 and a 1:1:1 triplet corresponding to HDO.