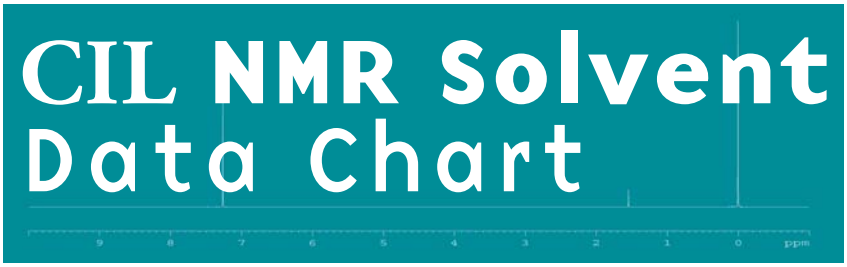
CIL NMR Solvent Data Chart



More Solvents, More Sizes, More Solutions

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)	 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) 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	1.03	-61	153	36.7	80.14
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) 3.56 (1) 1.11 (m)		 56.96 (5) 17.31 (7)	 22 19	5.3	0.89	-114.1	78.5	24.5	52.11
Methanol-d_4	4.78 (1) 3.31 (5)	 1.7	 49.15 (7)	 21.4	4.9	0.89	-97.8	64.7	32.7	36.07
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) 7.58 (1) 7.22 (1)		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	5	1.05	-42	115-116	12.4	84.13
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) 1.73 (1)		67.57 (5) 25.37 (5)	22.2 20.2	2.4-2.5	0.99	-108.5	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	110.6	2.4	100.19
Trifluoroacetic Acid-d	11.50 (1)		164.2 (4) 116.6 (4)		11.5	1.41	-15.4	72.4		115.03
Trifluoroethanol-d_3	5.02 (1) 3.88 (4x3)	 2(9)	126.3 (4) 61.5 (4x5)	 22	5	1.41	-43.3	75		103.06

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.

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■ 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.

NMR Solvent Storage and Handling Information

Acetic Acid-d_4	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Acetone-d_6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Acetonitrile-d_3	Store at room temperature away from light and moisture. Stable for one year after receipt of order if stored under above conditions (unopened). After one year, the compound should be re-checked for chemical purity before use.
Benzene-d_6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Chloroform-d	Store refrigerated (-5° to 5°C) away from light and moisture. Stable for six months after receipt of order if stored under above conditions (unopened). After six months, the compound should be re-checked for chemical purity before use.
Cyclohexane-d_{12}	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Deuterium Oxide	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
N,N-Dimethylformamide-d_7	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Dimethyl Sulfoxide-d_6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
1,4-Dioxane-d_8 (p-Dioxane)	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Ethanol-d_6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Methanol-d_4	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Methylene Chloride-d_2	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Pyridine-d_5	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
1,1,2,2-Tetrachloroethane-d_2	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Tetrahydrofuran-d_8	Store refrigerated (-5° to 5°C) away from light and moisture. Stable for six months after receipt of order if stored under above conditions (unopened). After six months, the compound should be re-checked for chemical purity before use.
Toluene-d_8	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Trifluoroacetic Acid-d	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
2,2,2-Trifluoroethanol-d_3	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.

Please note that some packaging sizes of some solvents may require special handling not given above. The bottle or ampule packaging should be checked for further instructions.

CIL

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