

Common NMR Solvents - Reference Data

Solvent	¹ H Chemical Shift	JHD (Hz)	¹³ C Chemical Shift	JCD (Hz)	¹ H Chemical Shift of HOD	Density at 20°C	Melting Point (°C)	Boiling Point (°C)	Dielectric Constant	Molecular Weight
Acetic Acid-d4	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-d6	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-d3	1.94 (5)	2.5	118.69 (1) 1.39 (7)	21	2.1	0.84	-45	81.6	37.5	44.07
Benzene-d6	7.16 (1)	-	128.39 (3)	24.3	0.4	0.95	5.5	80.1	2.3	84.15
Chloroform-d1 CDCl3	7.24 (1)	-	77.23 (3)	32.0	1.5	1.5	-63.5	61-62	4.8	120.38
Cyclohexane- d12	1.38 (1)	-	26.43 (5)	19	0.8	0.89	6.47	80.7	2	96.24
D2O	4.80 (DSS) 4.81 (TSP)	-	NA	NA	4.8	1.11	3.81	101.42	78.5	20.03
DMSO-d6	2.50 (5)	1.9	39.51 (7)	21.0	3.3	1.19	18.45	189	46.7	84.17
Dioxane-d8	3.53 (m)	-	66.66 (5)	21.9	2.4	1.13	11.8	101.1	2.2	96.16
Ethanol-d6	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-d4	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-d2	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	39.75	8.9	86.95
Pyridine-d5	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
THF-d8	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-d8	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

Notes: Adapted from the CIL NMR Solvent Data Chart.

Data originally taken from the Merck Index; S Budavari, et. al.

¹H and ¹³C spectra obtained at 200 MHz and 295°K.

²H is spin 1; triplets arising from coupling to ²H have an intensity ratio of 1:1:1.

'm' denotes a broad peak with some fine structure.

Chemical shifts may depend on solvent, concentration and temperature.

Melting and boiling points are for the unlabeled compound (except D2O).

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NMR Solvent Storage and Handling Information

Acetic Acid-d4	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Acetone-d6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Acetonitrile-d3	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.
C6D6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Chloroform-d1 CDCl3	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-d12	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
D2O	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
DMSO-d6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Dioxane-d8	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Ethanol-d6	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Methanol-d4	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Methylene Chloride-d2	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
Pyridine-d5	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.
THF-d8	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-d8	Store at room temperature away from light and moisture. Stable if stored under recommended conditions.

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