UNIVERSITY OF Southampton
School of Chemistry

Properties of Selected Deuterated Solvents for NMR Spectroscopy

Solvent	M_r	MP [°C]	BP [°C]	^{1}H shift (Mult.) [ppm]	J_{HD} [Hz]	^{13}C shift (Mult.) [ppm]	J_{CD} [Hz]	H_2O/ HOD shift [ppm]
Acetone-d_6	64.12	-93.8	55.5	2.05 (5)	2.2	29.92 (7) 206.68 (13)	19.4 0.9	2.84/ 2.81
Acetonitrile-d_3	44.07	-46	80.7	1.94 (5)	2.5	1.39 (7) 118.69	21	2.12
Benzene-d_6	84.15	6.8	79.1	7.16		128.39 (3)	24.3	0.4
Chloroform-d	120.38	-64.1	60.9	7.24		77.23 (3)	32	1.55
Deuterium Oxide	20.03	3.8	101.4	4.81				
Dichloromethane-d_2	86.95	-97	39.5	5.32 (3)	1.1	54 (5)	27.2	1.52
Diethylether-d_{10}	84.19	-116.3	34.6	3.34 (m) 1.07 (m)		65.3 (5) 14.5 (7)	21 19	
N,*N*-dimethyl-formamide-d_7	80.14	-60	153	8.03 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	3.45
Dimethylsulfoxide-d_6	84.17	20.2	190	2.50 (5)	1.9	39.51 (7)	21.0	3.3
1,4-dioxane-d_6	96.16	12	99	3.53 (m)		66.66 (5)	21.9	2.4
Ethanol-d_6	52.11	-114.5	78	5.29 3.56 1.11 (m)		 56.96 (5) 17.31 (7)	 22 19	5.2
Methanol-d_4	36.07	-99	65	4.87 3.31 (5)	 1.7	 49.15 (7)	 21.4	4.86
Nitrobenzene-d_5	128.14	6	211	8.11 (br) 7.67 (br) 7.50 (br)		148.6 134.8 (3) 129.5 (3) 123.5 (3)	 24.5 25 26	2.42
Nitromethane-d_3	64.06	-26	100	4.33 (5)		62.8 (7)	22	2.2
Pyridine-d_5	84.13	-41	114	8.74 7.58 7.22		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	4.97
Tetrahydrofuran-d_8	80.16	-108	64	3.58 1.73		67.57 (5) 25.37 (5)	22.2 20.2	2.42
Toluene-d_8	100.19	-85	109	 7.09 (m) 7.00 6.98 (m) 2.09 (5)	 2.3	137.86 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	 23 24 24 19	0.45
2,2,2-Trifluoroacetic acid-d	115.03	-15	71	11.50		164.2 (4) 116.6 (4)		11.5
2,2,2-Trifluoro-ethanol-d_3	87.06	-44	77	5.02 3.88 (4x3)	 2 (9)	126.3 (4) 61.5 (4x5)	 22	5

Taken from the Bruker almanac 2009