DEUTERATED NMR SOLVENTS - HANDY REFERENCE DATA

Compound Mol. Wt.	d_4^{20}	m.p.[a]	b.p.[a]	δ_H(mult)[b]	J_{HD}	δ_C(mult)[b]	$J_{CD}(J_{CF})$
Acetic Acid-d_4 64.078	1.12	17	118	11.53(1) 2.03(5)	2	178.4(br) 20.0(7)	 20
Acetone-d_6 64.177	0.87	-94	57	 2.04(5)	 2.2	206.0(13) 29.8(7)	0.9 20
Acetonitrile-d_3 44.071	0.84	-45	82	 1.93(5)	 2.5	118.2(br) 1.3(7)	 21
Benzene-d_6 84.152	0.95	5	80	7.15(br)		128.0(3)	24
Chloroform-d 120.384	1.50	-64	62	7.24(1)		77.0(3)	32
Cyclohexane-d_{12} 96.236	0.89	6	81	1.38(br)		26.4(5)	19
Deuterium Oxide 20.028	1.11	3.8	101.4	4.63(DSS) 4.67(TSP)			
1,2-Dichloroethane-d_4 102.985	1.25	-40	84	3.72(br)		43.6(5)	23.5
Diethyl-d_{10} Ether 84.185	0.82	-116	35	3.34(m) 1.07(m)		65.3(5) 14.5(7)	21 19
Diglume-d_{14} 148.263	0.95	-68	162	3.49(br) 3.40(br) 3.22(5)	 1.5	70.7(5) 70.0(5) 57.7(7)	21 21 21
Dimethylformamide-d_7 80.138	1.04	-61	153	8.01(br) 2.91(5) 2.74(5)	 2 2	162.7(3) 35.2(7) 30.1(7)	30 21 21
Dimethyl-d_6 Sulphoxide 84.170	1.18	18	189	2.49(5)	1.7	39.5(7)	21
p-Dioxane-d_8 96.158	1.13	12	101	3.53(m)		66.5(5)	22
Ethyl Alcohol-d_6 (anh) 52.106	0.91	<-130	79	5.19(1) 3.55(br) 1.11(m)		 56.8(5) 17.2(7)	 22 19
Glyme-d_{10} 100.184	0.86	-58	83	3.40(m) 3.22(5)	 1.6	71.7(5) 57.8(7)	21 21
Hexafluoroacetone Deuterate[c] 198.067	1.71	21		5.26(1)		122.5(4) 92.9(7)	(287) (34.5)
HMPT-d_{18} 197.314	1.14	7	106(11)	2.53(2x5)	2(9.5)	35.8(7)	21

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Methyl Alcohol-d_4	0.89	-98	65	4.78(1)		49.0(7)	21.5
36.067				3.30(5)	1.7		
Methylene Chloride-d_2	1.35	-95	40	5.32(3)	1	53.8(5)	27
86.945							
Nitrobenzene-d_5	1.25	6	211			148.6(1)	
128.143				8.11(br)		134.8(3)	24.5(p)
				7.67(br)		129.5(3)	25
				7.50(br)		123.5(3)	26
Nitromethane-d_3	1.20	-29	101	4.33(5)	2	62.8(7)	22
64.059							
isoPropyl Alcohol-d_8	0.90	-86	83	5.12(1)			
68.146				3.89(br)		62.9(3)	21.5
				1.10(br)		24.2(7)	19
Pyridine-d_5	1.05	-42	116	8.71(br)		149.9(3)	27.5
84.133				7.55(br)		135.5(3)	24.5(γ)
				7.19(br)		123.5(3)	25
Tetrahydrofuran-d_8	0.99	-109	66	3.58(br)		67.4(5)	22
80.157				1.73(br)		25.3(br)	20.5
Toluene-d_8	0.94	-95	111			137.5(1)	
100.191				7.09(m)		128.9(3)	23
				7.00(br)		128.0(3)	24
				6.98(m)		125.2(3)	24(p)
				2.09(5)	2.3	20.4(7)	19
Trifluoroacetic Acid-d[d]	1.50	-15	72	11.50(1)		164.2(4)	(44)
115.030						116.6(4)	(283)
2,2,2-Trifluoroethyl Alcohol-d_3	1.45	-44	75	5.02(1)		126.3(4)	(277)
103.059				3.88(4x3)	2(9)	61.5(4x5)	22(36)

[a]Melting and boiling points (in °C) are those of the corresponding light compound (except for D_2O) and are intended only to indicate the useful liquid range of the materials.

[b]^1H (of the residual protons) and ^{13}C spectra were determined on HA-100 and XL-100-15 spectrometers, respectively, for the same sample of each solvent containing 5% TMS (v/v). The chemical shifts are in ppm relative to TMS; the coupling constants are in Hz. (Since deuterium has a spin of 1, triplets arising from coupling to deuterium have the itensity ratio of 1:1:1, etc.) The multiplicity br indicates a broad peak without resolvable fine structure, while m denotes one with fine structure. It should be noted that the chemical shifts, in particular, can be dependent on solute, concentration and temperature.

[c]$\delta_F(CFCl_3)$82.6(1) [d]$\delta_F(CFCl_3)$76.2(1) [e]$\delta_F(CFCl_3)$77.8(5), J_{FD} 1.2 all determined on an HA-100 spectrometer.