DEUTERATED NMR SOLVENTS-HANDY REFERENCE DATA

Compound Mol. Wt.	d_4^{20}	m.p.*	b.p.*	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 64.117	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
Diglyme-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 96.156	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(2 x 5)	2 (9.5)	35.8 (7)	21
Methyl Alcohol-d_4 36.067	0.89	-98	65	4.78 (1) 3.30 (5)	 1.7	49.0 (7)	21.5
Methylene Chloride-d_2 86.945	1.35	-95	40	5.32 (3)	1	53.8 (5)	27
Nitrobenzene-d_5 128.143	1.25	6	211	 8.11 (br) 7.67 (br) 7.50 (br)	 	148.6 (1) 134.8 (3) 129.5 (3) 123.5 (3)	 24.5 (p) 25 26
Nitromethane-d_3 64.059	1.20	-29	101	4.33 (5)	2	62.8 (7)	22
isoPropyl Alcohol-d_8 68.146	0.90	-86	83	5.12 (1) 3.89 (br) 1.10 (br)	 	 62.9 (3) 24.2 (7)	 21.5 19
Pyridine-d_5 84.133	1.05	-42	116	8.71 (br) 7.55 (br) 7.19 (br)	 	149.9 (3) 135.5 (3) 123.5 (3)	27.5 24.5 (γ) 25
Tetrahydrofuran-d_8 80.157	0.99	-109	66	3.58 (br) 1.73 (br)	 	67.4 (5) 25.3 (br)	22 20.5
Toluene-d_8 100.191	0.94	-95	111	 7.09 (m) 7.00 (br) 6.98 (m) 2.09 (5)	 2.3	137.5 (1) 128.9 (3) 128.0 (3) 125.2 (3) 20.4 (7)	 23 24 24 (p) 19
Trifluoroacetic Acid-d[d] 115.030	1.50	-15	72	11.50 (1)		164.2 (4) 116.6 (4)	(44) (283)
2,2,2-Trifluoroethyl Alcohol-d_3[e] 103.059	1.45	-44	75	5.02 (1) 3.88(4 x 3)	 2 (9)	126.3 (4) 61.5(4 x 5)	(277) 22 (36)

*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 intensity 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.

MERCK & CO., Inc.
ISOTOPES
4545 OLEATHA AVE.
ST. LOUIS, MO 63116
314 353-7000
800 325-9034
P.O. BOX 2951 TERMINAL ANNEX
LOS ANGELES, CA 90051
213 723-9521
MERCK SHARP & DOHME
ISOTOPES
P.O. BOX 899
POINTE CLAIRE-DORVAL
QUEBEC H9R 4P7
514 697-2823