Table 4.A.1: Commonly Used Deuterated Solvents[a]

Adapted from the AM Series User's Manual (4-6)

Name	formula	^{1}H (ppm) *	Multiplicity*	^{13}C (ppm)	Multiplicity
Acetone-d_6	CD_3COCD_3	2.04	Quintet (5)	29.8 ($^{13}CD_3$'s) 206 (^{13}C=O)	(13) 7
Benzene-d_6	C_6D_6	7.15	1 (broad)	128.0	3
Chloroform-d	$CDCl_3$	7.24	1	77.0	3
D_2O	D_2O	4.60 / 4.79[c]	1	----	----
DMSO-d_6	CD_3SOCD_3	2.49	5	39.5	7
MeOH-d_4	CD_3OD	4.78 (O^1H) 3.30[b] (C^1HD_2)	1 5[b]	49.0	7
Methylene Chloride-d_2	CD_2Cl_2	5.32	3	53.8	5
Pyridine-d_5	C_5D_5N	8.71 7.55 7.19	1 (broad) 1 (broad) 1 (broad)	149.9 135.5 123.5	3 3 3
THF	$(CD_2)_4O$	3.58[b] -O-C^1HD-CD_2- 1.73[b] -CD_2-C^1HD-CD_2	1 (broad) 1 (broad)	67.4[b] -O-$^{13}CD_2$-CD_2- 25.3[b] -CD_2-$^{13}CD_2$-CD_2	5 1 (broad)
Toluene-d_8	Ph-CD_3	6.98 to 7.09 (Ph) 2.09[a] (C^1HD_2)	1 5	137.5[b] (>^{13}C-CD_3) 125-129[b] (o,m,p) 20.4[b] ($^{13}CD_3$)	1 3 7

[*] **of residual proton signal in deuterated solvent**

[a] relative to TMS = 0 ppm CHEMICAL SHIFTS CAN VARY WITH ***SOLUTE***, ***CONCENTRATION***, AND ***TEMPERATURE***.

[b] Merck & Co., Inc. Isotopes, Handy Reference Data

[c] ***J Org Chem*** **62:7513-7514 (1997) (Tables 1 & 2, includes J couplings)**

SEE ALSO http://riodb.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng