参考資料

参考資料 9

Table 1.1H NMR Data

	proton	mult	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
Solvent Residual Peak			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O		s	1.56	2.84 [a]	3.33 [a]	0.40	2.13	4.87	-
Acetic acid	CH_3	s	2.10	1.96	1.91	1.55	1.96	1.99	2.08
Acetone	CH_3	s	2.17	2.09	2.09	1.55	2.08	2.15	2.22
Acetonitrile	CH_3	s	2.10	2.05	2.07	1.55	1.96	2.03	2.06
Benzene	CH	s	7.36	7.36	7.37	7.15	7.37	7.33	-
tert-Butyl alcohol	CH_3	s	1.28	1.18	1.11	1.05	1.16	1.40	1.24
	OHc	s	-	-	4.19	1.55	2.18	-	-
tert-Butyl methyl ether	CCH_3	s	1.19	1.13	1.11	1.07	1.14	1.15	1.21
	OCH_3	s	3.22	3.13	3.08	3.04	3.13	3.20	3.22
Chloroform	CH	s	7.26	8.02	8.32	6.15	7.58	7.90	-
Cyclohexane	CH_2	s	1.43	1.43	1.40	1.40	1.44	1.45	-
1,2-Dichloroethane	CH_2	s	3.73	3.87	3.90	2.90	3.81	3.78	-
Dichloromethane	CH_2	s	5.30	5.63	5.76	4.27	5.44	5.49	-
Diethyl ether	CH_3	t,7	1.21	1.11	1.09	1.11	1.12	1.18	1.17
	CH_2	q,7	3.48	3.41	3.38	3.26	3.42	3.49	3.56
1,2-Dimethoxyethane	CH_3	s	3.40	3.28	3.24	3.12	3.28	3.35	3.37
	CH_2	s	3.55	3.46	3.43	3.33	3.45	3.52	3.60
Dimethylformamide	CH	s	8.02	7.96	7.95	7.63	7.92	7.97	7.92
	CH_3	s	2.96	2.94	2.89	2.36	2.89	2.99	3.01
	CH_3	s	2.88	2.78	2.73	1.86	2.77	2.86	2.85
Dimethyl sulfoxide	CH_3	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
Dioxane	CHz	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
Ethanol	CH_3	t,7	1.25	1.12	1.06	0.96	1.12	1.19	1.17
	CH_2	q,7 [c]	3.72	3.57	3.44	3.34	3.54	3.60	3.65
	OH	s [b,c]	1.32	3.39	4.63	-	2.47	-	-
Ethyl acetate	CH_3CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH_2CH_3	q,7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH_2CH_3	t,7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
Ethyl methyl ketone	CH_3CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH_2CH_3	q,7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH_2CH_3	t,7	1.06	0.96	0.91	0.85	0.96	1.01	1.26
Ethylene glycol	CH	s [d]	3.76	3.28	3.34	3.41	3.51	3.59	3.65
n-Hexane	CH_3	t	0.88	0.88	0.86	0.89	0.89	0.90	-
	CH_2	m	1.26	1.28	1.25	1.24	1.28	1.29	-
Methanol	CH_3	s [e]	3.49	3.31	3.16	3.07	3.28	3.34	3.34
	OH	s [b,e]	1.09	3.12	4.01	-	2.16	-	-
Nitromethane	CH_3	s	4.33	4.43	4.42	2.94	4.31	4.34	4.40
n-Pentane	CH_3	t,7	0.88	0.88	0.86	0.87	0.89	0.90	-
	CH_2	m	1.27	1.27	1.27	1.23	1.29	1.29	-
Pyridine	CH(2)	m	8.62	8.58	8.58	8.53	8.57	8.53	8.52
	CH(3)	m	7.29	7.35	7.39	6.66	7.33	7.44	7.45
	CH(4)	m	7.68	7.76	7.79	6.98	7.73	7.85	7.87
Tetrahydrofuran	CH_2	m	1.85	1.79	1.76	1.40	1.80	1.87	1.88
	CH_2O	m	3.76	3.63	3.60	3.57	3.64	3.71	3.74
Toluene	CH_3	s	2.36	2.32	2.30	2.11	2.33	2.32	-
	CH(o/p)	m	7.17	7.1-7.2	7.18	z	7.1-7.3	7.16	-
	CH(m)	m	7.25	7.1-7.2	7.25	7.13	7.1-7.3	7.16	-
Triethylamine	CH_3	t,7	1.03	0.96	0.93	0.96	0.96	1.05	0.99
	CH_2	q,7	2.53	2.45	2.43	2.40	2.45	2.58	2.57

a In these solvents the intermolecular rate of exchange is slow enough that a peak due to HDO is usually also observed; it appears at 2.81 and 3.30 ppm in acetone and DMSO, respectively.
In the former solvent. it is often seen as a 1:1:1 triplet, with 2JH.D = 1 Hz.

b The signals from exchangeable protons were not always identified.

c In some cases (see note a), the coupling interaction between the CH_2 and the OH protons may be observed (J = 5 Hz).

d In CD_3CN, the OH proton was seen as a multiplet at δ 2.69, and extra coupling was also apparent on the methylene peak.

e In some cases (see notes a, d), the coupling interaction between the CH_3 and the OH protons may be observed (J = 5.5 Hz),