

Common ¹H NMR Impurities

From *J. Org. Chem.*, 62, 1997 and additional sources

SOLVENT	CDCl ₃	Acetone	DMSO	C ₆ D ₆	CD ₃ CN	MeOD	D ₂ O
Residual Solvent Peak	7.26	2.05	2.50	7.16	1.94	3.31	4.79
Acetic Acid	2.13 11.53	1.96	1.91	1.55	1.96	1.99	2.08
Acetone	2.17	2.09	2.09	1.55	2.08	2.15	2.22
Acetonitrile	2.10	2.05	2.07	1.55	1.96	2.03	2.06
Benzene	7.36	7.36	7.37	7.15	7.37	7.33	
Benzyl alcohol	4.72						
Benzyl bromide	7.39 (m) 7.47 (d) 4.50 (s)						
BHT	6.98 5.01 2.27 1.43	6.96 - 2.22 1.41	6.87 6.65 2.18 1.36	7.05 4.79 2.24 1.38	6.97 5.20 2.22 1.39	6.92 - 2.21 1.40	
Bromoform	6.85	-	7.75			7.42	insol
n-Butanol	3.67 (t, 6) 0.94 (t, 7) 4.56 (s)	-	3.41 0.89			3.54 0.93	3.60 0.89
t-Butanol	1.28	1.18	1.11 (s) 4.19 (br s)	1.05 (s) 1.55 (br s)	1.16 (s) 2.18 (br s)	1.40	1.24
t-Butyl methyl ether	1.19 3.22	1.13 3.13	1.11 3.08	1.07 3.04	1.14 3.13	1.15 3.20	
Chloroacetic acid	4.14	-	4.28			-	4.25
Chloroform	7.26	8.02	8.32	6.15	7.58	7.90	insol
Cyclohexane	1.43	1.43	1.40	1.40	1.44	1.45	insol
1,2-Dibromoethane	3.63	-	3.84			3.72	3.79
Dichoroacetic acid	5.98	-	6.68			-	6.21
1,2-Dichloroethane	3.73	3.87	3.90	2.90	3.81	3.78	3.92
Dichloromethane	5.30	5.63	5.76	4.27	5.44	5.49	insol
Diethyl ether	3.48 (q, 7) 1.20 (t, 7)	3.41 1.11	3.38 1.09	3.26 1.11	3.42 1.12	3.49 1.18	3.56 1.17
Diglyme	3.65 (m) 3.57 (m)	3.56 3.47	3.51 3.38	3.46 3.34	3.53 3.45	3.61 3.58	3.67 3.61
Diisopropyl ether	1.12 (d, 6)	-	1.04			-	1.12
Dimethoxyethane	3.40 (s) 3.55 (s)	3.28 3.46	3.24 3.43	3.12 3.33	3.28 3.45	3.35 3.52	3.37 3.60
Dimethylacetamide (DMA)	3.02 2.94 2.08	3.00 2.83 1.97	2.94 2.78 1.96	2.57 2.05 1.60	2.96 2.83 1.97	3.31 2.92 2.07	3.06 2.90 2.08
DMF	8.02 2.96 2.88	2.94 2.78 7.96	7.95 2.89 2.73	7.63 2.36 1.86	7.92 2.89 2.77	7.97 2.99 2.86	7.92 3.01 2.85
DMSO	2.62	2.52	2.54	1.68	2.50	2.65	2.71
Dioxan	3.71	3.59	3.57	3.35	3.60	3.66	3.75
Ethylene glycol	3.76	3.28	3.34	3.41	3.51	3.59	3.65
EtOH	3.72 (q, 7) 1.25 (t, 7) 1.32 (br)	3.57 1.12 3.39	3.44 1.06 4.63	3.34 0.96	3.54 1.12 2.47	3.60 1.19	3.65 1.17
Ethyl acetate	4.12 (q, 7) 2.04 (s) 1.26 (t, 7)	4.05 1.97 1.20	4.03 1.99 1.17	3.89 1.65 0.92	4.06 1.97 1.20	4.09 2.01 1.24	4.14 2.07 1.24
Ethyl formate	8.04 4.22 (q, 7) 1.29 (t, 7)	-	8.23 4.17 1.24			- - -	8.16 4.28 1.29
Ethyl methyl ketone	2.14 (s) 2.46 (q) 1.06 (t)	2.07 2.45 0.96	2.07 2.43 0.91	1.58 1.81 0.85	2.06 2.43 0.96	2.12 2.50 1.01	2.19 3.18 1.26

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SOLVENT	CDCl ₃	Acetone	DMSO	C ₆ D ₆	CD ₃ CN	MeOD	D ₂ O
Formic acid	2.12	-	2.08			-	2.19
<i>n</i> -Hexane	0.88 (t) 1.26 (m)	0.88 1.26	0.86 1.25	0.89 1.24	0.89 1.28	0.90 1.29	
Isobutyl methyl ketone	2.12 0.92 (d, 6)	-	2.08 0.88			2.11 0.91	2.19 0.88
Isopropyl acetate	2.02 1.22 (d, 6)	-	2.00 1.21			1.99 1.22	Insol
Isopropyl alcohol	4.04 (m) 1.22 (d, 6)	3.90 1.10	3.78 1.04	3.67 0.95	3.87 1.09	3.92 1.50	4.02 1.17
MeOH	3.49 1.09 (br)	3.31 3.12	3.16 4.01	3.07	3.28 2.16	3.34	3.34
Methyl acetate	3.67 2.05	-	3.61 1.92			-	3.68 2.09
Methyl iodide	2.16	-	2.21			2.15	Insol
Morpholine	3.69 (m) 2.85 (m)	-	3.52 2.68			3.64 2.79	3.70 2.79
Nitromethane	4.32	-	4.44			-	4.41
NMP	3.39 (t), 2.85 (s), 2.38 (t), 2.02 (m)	-	-			-	-
<i>n</i> -Pentane	0.88 (t) 1.27 (m)	0.88 1.27	0.86 1.27	0.87 1.23	0.89 1.29	0.90 1.29	
Petroleum spirit (60 ° - 80 °)	1.28 0.90	-	1.28 0.89			1.30 0.88	Insol
Potassium acetate	insol	-	1.60			-	1.91
Propanol	3.60 (t, 7) 1.60 (m) 0.93 (t, 7)	-	1.45 0.87			3.49 1.54 0.92	3.61 1.57 0.89
Propionic acid	2.42 (q, 7) 1.18 (t, 7)	-	2.26 1.03			-	2.47 1.10
Pyridine	8.62 (m) 7.68 (m) 7.29 (m)	8.58 7.76 7.35	8.58 7.79 7.39	8.53 6.98 6.66	8.57 7.73 7.33	8.53 7.85 7.44	8.52 7.87 7.45
Pyridine HCl		-				8.92, 8.19, 8.69	
Succinimide	2.77 8.9	-	2.63			-	2.78
TCE (1,1,2,2-tetrachloroethane)	6.0						
THF	3.76 (m) 1.85 (m)	3.63 1.79	3.60 1.76	3.57 1.40	3.64 1.80	3.71 1.87	3.74 1.88
Toluene	7.17 (m) 7.25 (m) 2.36	7.1 – 7.2 2.32	7.18 7.25 2.30	7.02 7.13 2.11	7.1 – 7.3 2.33	7.16 7.16 2.33	Insol
1,1,1 -Trichloroethane	2.72	-	2.80			insol	Insol
Triethylamine	2.53 (q, 7) 1.03 (t, 7)	2.45 0.96	2.43 0.93	2.40 0.96	2.45 0.96	2.58 1.05	2.57 0.99
Triethylamine HCl	3.03 (q) 1.32 (t)	-				3.23 (q, 7) 1.34 (t, 7)	
Trifluoroethanol	5.02 3.88						
Water	1.58	2.83	3.33	0.40	2.13	4.87	4.76
“grease” long chain alkanes	1.26 (br s) 0.86 (m)	1.29 0.87		1.36 0.92	1.27 0.86	1.20 0.88	
Silicone grease	0.07 (s)	0.13		0.29	0.08	0.10	