NMR Chemical Shifts of Common Solvents as Trace Impurities

^{1}H NMR Chemical Impurity Shifts Table

	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	3.33	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	7.36	7.15	7.37	7.33	
Benzyl alcohol	CH CH CH_2 OH	m m d, 5.9 t, 5.9	7.28–7.38 7.28–7.38 4.71 1.64	7.29–7.37 7.20–7.25 4.63 4.16	7.28–7.36 7.20–7.25 4.49 5.16		7.30–7.37 7.23–7.29 4.57 3.14	7.30–7.36 7.22–7.26 4.59, s	7.37–7.47 7.37–7.47 4.65, s
***tert*-Butanol**	CH_3 OH	s s	1.27	1.18 3.22	1.11 4.18	1.05 1.55	1.17 2.39	1.22	1.25
2-Butanone (MEK)	CH_3CO CH_2 CH_2CH_3	s q, 7 t, 7	2.14 2.46 1.06	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
***tert*-Butyl methyl ether (MTBE)**	CCH_3 OCH_3	s s	1.19 3.22	1.13 3.13	1.11 3.08	1.07 3.04	1.14 3.13	1.15 3.20	1.21 3.22
Chlorobenzene	CH	m	7.22–7.36	7.31–7.42	7.32–7.45		7.29–7.41	7.25–7.37	7.33–7.46
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	
Cyclopentyl methyl ether (CPME)	CH OCH_3 CH_2	m s m	3.78–3.82 3.28 1.50–1.74	3.73–3.77 3.19 1.44–1.72	3.71–3.76 3.15 1.42–1.67		3.74–3.78 3.19 1.48–1.70	3.80–3.85 3.26 1.50–1.77	3.94–3.99 3.30 1.51–1.86
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 CH_2	t, 7 q, 7	1.21 3.48	1.11 3.41	1.09 3.38	1.11 3.26	1.12 3.42	1.18 3.49	1.17 3.56
1,2-Dimethoxyethane	CH_3 CH_2	s s	3.40 3.55	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	CH_3CO NCH_3 NCH_3	s s s	2.09 3.02 2.94	1.97 3.00 2.83	1.96 2.94 2.78	1.60 2.54 2.05	1.97 2.96 2.83	2.07 3.30 2.92	2.08 3.06 2.90
Dimethylformamide	CH CH_3 CH_3	s s s	8.02 2.96 2.88	7.96 2.94 2.78	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
Dimethyl sulfoxide	CH_3	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
Dioxane	CH_2	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
Ethanol	CH_3 CH_2 OH	t, 7 q, 7 s	1.25 3.72 1.32	1.12 3.57 3.39	1.06 3.44 4.63	0.96 3.34	1.12 3.54 2.47	1.19 3.60	1.17 3.65
Ethyl acetate	CH_3CO CH_2CH_3 CH_2CH_3	s q, 7 t, 7	2.05 4.12 1.26	1.97 4.05 1.20	1.99 4.03 1.17	1.65 3.89 0.92	1.97 4.06 1.20	2.01 4.09 1.24	2.07 4.14 1.24
Ethylene glycol	CH	s	3.67	3.28	3.34	3.41	3.51	3.59	3.65
Grease	CH_3 CH_2	m brs	0.86 1.26	0.87 1.29		0.92 1.36	0.86 1.27	0.88 1.29	
***n*-Hexane**	CH_3 CH_2	t m	0.88 1.26	0.88 1.28	0.86 1.25	0.89 1.24	0.89 1.28	0.90 1.29	
Methanol	CH_3 OH	s s	3.49 1.09	3.31 3.12	3.16 4.01	3.07	3.28 2.16	3.34	3.34
Nitromethane	CH_3	s	4.33	4.43	4.42	2.94	4.31	4.34	4.40
***n*-Pentane**	CH_3 CH_2	t, 7 m	0.88 1.27	0.88 1.27	0.86 1.27	0.87 1.23	0.89 1.29	0.90 1.29	
2-Propanol	CH CH_3 OH	septd, 6.1, 4.3 d, 6.1 d, 4.3	4.03, sept (6.1) 1.21	3.84–3.95, m 1.10 3.39	3.77 1.04 4.34		3-89 1.09 2.51	3.92, sept (6.1) 1.15	4.02, sept (6.2) 1.18
Pyridin	CH (2) CH (3) CH (4)	m m m	8.62 7.29 7.68	8.58 7.35 7.76	8.58 7.39 7.79	8.53 6.66 6.98	8.57 7.33 7.73	8.53 7.44 7.85	8.52 7.45 7.87
Silicone grease	CH_3	s	0.07	0.13		0.29	0.08	0.10	
Tetrahydrofuran	CH_2 CH_2O	m m	1.85 3.76	1.79 3.63	1.76 3.60	1.40 3.57	1.80 3.64	1.87 3.71	1.88 3.74
Toluene	CH_3 CH (*o*/*p*) CH (*m*)	s m m	2.36 7.17 7.25	2.32 7.1–7.2 7.1–7.2	2.30 7.18 7.25	2.11 7.02 7.13	2.33 7.1–7.3 7.1–7.3	2.32 7.16 7.16	
Triethylamine	CH_3 CH_2	t, 7 q, 7	1.03 2.53	0.96 2.45	0.93 2.43	0.96 2.40	0.96 2.45	1.05 2.58	0.99 2.57
Xylenes									
***o*-Xylene**	CH CH_3	m s	7.08–7.14 2.26	7.03–7.12 2.23	7.04–7.14 2.21		7.05–7.15 2.25	7.01–7.10 2.24	
***m*-Xylene**	CH (5) CH (2,4,6) CH_3	t, 7.5 m s	7.15 6.96–7.00 2.32	7.15 6.94–6.99 2.27	7.13 6.95–6.99 2.26		7.13 6.96–7.01 2.28	7.08 6.92–6.97 2.27	7.24 7.07–7.14 2.31
***p*-Xylene**	CH CH_3	s s	7.06 2.31	7.05 2.26	7.05 2.24		7.06 2.27	7.02 2.26	7.18 2.30

References

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Please note that the values given in the tables are temperature- and partly concentration-dependent and therefore represent average values only.

^{13}C NMR Chemical Impurity Shifts Table

	Carbon	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
Solvent residual peak		77.16 ±0.06	29.84 ±0.01 206.26 ±0.13	39.52 ±0.06	128.06 ±0.02	1.32 ±0.02 118.26 ±0.02	49.00 ±0.01	
Acetic acid	CO CH_3	175.99 20.81	172.31 20.51	171.93 20.95	175.82 20.37	173.21 20.73	175.11 20.56	177.21 21.03
Acetone	CO CH_3	207.07 30.92	205.87 30.60	206.31 30.56	204.43 30.14	207.43 30.91	209.67 30.67	215.94 30.89
Acetonitrile	CN CH_3	116.43 1.89	117.60 1.12	117.91 1.03	116.20 0.20	118.26 1.79	118.06 0.85	119.68 1.47
Benzene	CH	128.37	129.15	128.30	128.62	129.32	129.34	
Benzyl alcohol	*C (1)* *CH (3,5)* *CH (4)* *CH (2,6)* *CH_2*	140.98 128.54 127.61 126.98 65.31	143.52 128.92 127.55 127.35 64.68	142.44 127.92 126.50 126.31 62.82		143.17 129.26 127.97 127.69 64.76	142.74 129.37 128.28 128.01 65.28	140.84 129.34 128.43 128.06 64.51
***tert*-Butanol**	C CH_3	69.15 313.25	68.13 30.72	66.88 30.88	68.19 30.47	68.74 30.68	69.40 30.91	70.36 30.29
2-Butanone (MEK)	CH_3CO CO CH_2 CH_2CH_3	29.49 209.56 36.89 7.86	29.30 208.30 36.75 8.03	29.26 208.70 35.83 7.61	28.56 206.55 36.36 7.91	29.60 209.88 37.09 8.14	29.39 212.16 37.34 8.09	29.49 218.43 37.27 7.87
***tert*-Butyl methyl ether (MTBE)**	OCH_3 C CCH_3	49.45 72.87 26.99	49.35 72.81 27.24	48.70 72.04 26.79	49.19 72.40 27.09	49.52 73.17 27.28	49.66 74.32 27.22	49.37 75.62 26.60
Chlorobenzene	C (1) CH (3,5) CH (2,6) CH (4)	134.29 129.71 128.62 126.43	134.63 130.94 129.30 127.65	133.00 130.20 128.30 126.92		134.74 131.10 129.45 127.83	135.31 131.00 129.56 127.73	
Chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
Cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96	
Cyclopentyl methyl ether (CPME)	CH CH_3 CH_2 (2,5) CH_2 (3,4)	83.03 54.30 31.97 23.55	83.35 56.18 32.51 24.14	81.92 55.47 31.35 23.05		83.62 56.38 32.63 24.28	84.47 56.55 32.85 24.45	84.40 56.04 31.87 23.61
1,2-Dichloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11	
Dichloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78	
Diethyl ether	CH_3 CH_2	15.20 65.91	15.75 66.12	15.12 62.05	15.46 65.94	15.63 66.32	15.46 66.88	14.77 66.42
1,2-Dimethoxyethane	CH_3 CH_2	59.08 71.84	58.45 72.47	58.01 17.07	58.68 72.21	58.89 72.47	59.06 72.72	58.67 71.49
Dimethylacetamide	CH_3 CO NCH_3 NCH_3	21.53 171.07 35.28 38.13	21.51 170.61 34.89 37.92	21.29 169.54 37.38 34.42	21.16 169.95 34.67 37.03	21.76 171.31 35.17 38.26	21.32 173.32 35.50 38.43	21.09 174.57 35.03 38.76
Dimethylformamide	C CH_3 CH_3	162.62 36.50 31.45	162.79 36.15 31.03	162.29 35.73 30.73	162.13 35.25 30.72	163.31 36.57 31.32	164.73 36.89 31.61	165.53 37.54 32.03
Dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45	39.39
Dioxane	CH_2	67.14	67.60	66.36	67.16	67.72	68.11	67.19
Ethanol	CH_3 CH_2	18.41 58.28	18.89 57.72	18.51 56.07	18.72 57.86	18.80 57.96	18.40 58.26	17.47 58.05
Ethyl acetate	CH_3CO CO CH_2 CH_2	21.04 171.36 60.49 14.19	20.83 170.96 60.56 14.50	20.68 170.31 59.74 14.40	20.56 170.44 60.21 14.19	21.16 171.68 60.98 14.54	20.88 172.89 61.50 14.49	21.15 175.26 62.32 13.92
Ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30	63.17
Grease	CH_2	29.76	30.73	29.20	30.21	30.86	31.29	
***n*-Hexane**	CH_3 CH_2 (2) CH_2 (3)	14.14 22.70 31.64	14.34 23.28 32.30	13.88 22.05 30.95	14.32 23.04 31.96	14.43 23.40 32.36	14.45 23.68 32.73	
Methanol	CH_3	50.41	49.77	48.59	49.97	49.90	49.86	49.50
Nitromethane	CH_3	62.50	53.21	63.28	61.16	63.66	63.08	63.22
***n*-Pentane**	CH_3 CH_2 (2) CH_2 (3)	14.08 22.38 34.16	14.29 22.98 34.83	13.28 21.70 33.48	14.25 22.81 34.45	14.37 23.08 34.89	14.39 23.38 35.30	
2-Propanol	CH_3 CH	25.14 64.50	25.67 63.85	25.43 64.92	25.18 64.23	25.55 64.30	25.27 64.71	24.38 64.88
Pyridin	CH (2) CH (3) CH (4)	149.90 123.75 135.96	150.67 124.57 136.56	149.58 123.84 136.05	150.27 123.58 123.28	150.76 127.76 136.89	150.07 125.53 138.35	149.18 125.12 138.27
Silicone grease	CH_3	1.04	1.40		1.38		2.10	
Tetrahydrofuran	CH_2 CH_2O	25.62 67.97	26.15 68.07	25.14 67.03	25.72 67.80	26.27 68.33	26.48 68.83	25.67 68.68
Toluene	CH_3 CH (*i*) CH (*o*) CH (*m*) CH (*p*)	21.46 137.89 129.07 128.26 125.33	21.46 138.48 129.76 129.03 126.12	20.99 137.35 128.88 128.18 125.29	21.10 137.91 129.33 128.56 125.68	21.50 138.90 129.94 129.23 126.28	21.50 138.85 129.91 129.20 126.29	
Triethylamine	CH_3 CH_2	11.61 46.25	12.49 47.07	11.74 45.74	12.35 46.77	12.38 47.10	11.09 46.96	9.07 47.19
Xylenes								
***o*-Xylene**	C (1,2) CH (3,6) CH (4,5) CH_3	136.49 129.59 125.79 19.71	137.03 130.28 126.58 19.68	135.91 129.29 125.61 19.24		137.51 130.46 126.78 19.79	137.37 130.47 126.81 19.77	
***m*-Xylene**	C (1,3) CH (2) CH (5) CH (4,6) CH_3	137.78 129.91 128.15 126.04 21.33	138.34 130.52 128.93 126.78 21.32	137.07 129.51 127.98 125.83 20.83		138.80 130.71 129.16 126.95 21.40	138.79 130.70 129.13 126.99 21.42	
***p*-Xylene**	C (1,4) CH (2,3,5,6) CH_3	134.67 128.92 20.94	135.27 129.65 20.94	134.03 128.69 20.49		135.68 129.85 21.00	135.71 129.84 21.02	