

¹H NMR Chemical Impurity Shifts Table

	Proton	Mult.	CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
Solvent residual peak			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H ₂ O		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	m	7.28–7.38	7.29–7.37	7.28–7.36		7.30–7.37	7.30–7.36	7.37–7.47
	CH	m	7.28–7.38	7.20–7.25	7.20–7.25		7.23–7.29	7.22–7.26	7.37–7.47
	CH ₂	d, 5,9	4.71	4.63	4.49		4.57	4.59, s	4.65, s
	OH	t, 5,9	1.64	4.16	5.16		3.14		
tert-Butanol	CH ₃	s	1.27	1.18	1.11	1.05	1.17	1.22	1.25
	OH	s		3.22	4.18	1.55	2.39		
2-Butanone (MEK)	CH ₃ CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH ₂	q, 7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH ₂ CH ₃	t, 7	1.06	0.96	0.91	0.85	0.96	1.01	1.26
tert-Butyl methyl ether (MTBE)	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
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	m	3.78–3.82	3.73–3.77	3.71–3.76		3.74–3.78	3.80–3.85	3.94–3.99
	OCH ₃	s	3.28	3.19	3.15		3.19	3.26	3.30
	CH ₂	m	1.50–1.74	1.44–1.72	1.42–1.67		1.48–1.70	1.50–1.77	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	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
Dimethylacetamide	CH ₃ CO	s	2.09	1.97	1.96	1.60	1.97	2.07	2.08
	NCH ₃	s	3.02	3.00	2.94	2.54	2.96	3.30	3.06
	NCH ₃	s	2.94	2.83	2.78	2.05	2.83	2.92	2.90
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	CH ₂	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	3.72	3.57	3.44	3.34	3.54	3.60	3.65
	OH	s	1.32	3.39	4.63		2.47		
Ethyl acetate	CH ₃ CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH ₂ CH ₃	q, 7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH ₂ CH ₃	t, 7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
Ethylene glycol	CH	s	3.67	3.28	3.34	3.41	3.51	3.59	3.65
Grease	CH ₃	m	0.86	0.87		0.92	0.86	0.88	
	CH ₂	brs	1.26	1.29		1.36	1.27	1.29	
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	3.49	3.31	3.16	3.07	3.28	3.34	3.34
	OH	s	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	
2-Propanol	CH	septd, 6.1, 4.3	4.03, sept (6.1)	3.84–3.95, m	3.77		3.89	3.92, sept (6.1)	4.02, sept (6.2)
	CH ₃	d, 6.1	1.21		1.10		1.09	1.15	1.18
	OH	d, 4.3			3.39		4.34		
Pyridin	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
Silicone grease	CH ₃	s	0.07	0.13		0.29	0.08	0.10	
Tetrahydrofuran	CH ₂	m	1.85	1.79	1.76	1.40	1.80	1.87	1.88
	CH ₂ O	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	7.02	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
Xylenes									
o-Xylene	CH	m	7.08–7.14	7.03–7.12	7.04–7.14		7.05–7.15	7.01–7.10	
	CH ₃	s	2.26	2.23	2.21		2.25	2.24	
m-Xylene	CH (5)	t, 7.5	7.15	7.15	7.13		7.13	7.08	7.24
	CH (2,4,6)	m	6.96–7.00	6.94–6.99	6.95–6.99		6.96–7.01	6.92–6.97	7.07–7.14
	CH ₃	s	2.32	2.27	2.26		2.28	2.27	2.31
p-Xylene	CH	s	7.06	7.05	7.05		7.06	7.02	7.18
	CH ₃	s	2.31	2.26	2.24		2.27	2.26	2.30

References

1. Gottlieb, H. E.; Kotlyar, V.; Nudelman, A.; *J. Org. Chem.*, 1997, 62, 7512. 2. Babji, N. R.; McCusker, E. O.; Whiteker, G. T.; Canturk, B.; Choy, N.; Creemer, L. C.; Amicis, C. V. D.; Hewlett, N. M.; Johnson, P. L.; Knobelsdorf, J. A.; Li, F.; Lorsbach, B. A.; Nugent, B. M.; Ryan, S. J.; Smith, M. R.; Yang, Q. *Org. Process Res. Dev.* 2016, 20, 661–667.

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



¹³C NMR Chemical Impurity Shifts Table

	Carbon	CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
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)	140.98	143.52	142.44		143.17	142.74	140.84
	CH (3,5)	128.54	128.92	127.92		129.26	129.37	129.34
	CH (4)	127.61	127.55	126.50		127.97	128.28	128.43
	CH (2,6)	126.98	127.35	126.31		127.69	128.01	128.06
	CH ₂	65.31	64.68	62.82		64.76	65.28	64.51
tert-Butanol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH ₃	313.25	30.72	30.88	30.47	30.68	30.91	30.29
2-Butanone (MEK)	CH ₃ CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.70	206.55	209.88	212.16	218.43
	CH ₂	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH ₂ CH ₃	7.86	8.03	7.61	7.91	8.14	8.09	7.87
tert-Butyl methyl ether (MTBE)	OCH ₃	49.45	49.35	48.70	49.19	49.52	49.66	49.37
	C	72.87	72.81	72.04	72.40	73.17	74.32	75.62
	CCH ₃	26.99	27.24	26.79	27.09	27.28	27.22	26.60
Chlorobenzene	C (1)	134.29	134.63	133.00		134.74	135.31	
	CH (3,5)	129.71	130.94	130.20		131.10	131.00	
	CH (2,6)	128.62	129.30	128.30		129.45	129.56	
	CH (4)	126.43	127.65	126.92		127.83	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	83.03	83.35	81.92		83.62	84.47	84.40
	CH ₃	54.30	56.18	55.47		56.38	56.55	56.04
	CH ₂ (2,5)	31.97	32.51	31.35		32.63	32.85	31.87
	CH ₂ (3,4)	23.55	24.14	23.05		24.28	24.45	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	15.20	15.75	15.12	15.46	15.63	15.46	14.77
	CH ₂	65.91	66.12	62.05	65.94	66.32	66.88	66.42
1,2-Dimethoxyethane	CH ₃	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH ₂	71.84	72.47	17.07	72.21	72.47	72.72	71.49
Dimethylacetamide	CH ₃	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH ₃	35.28	34.89	37.38	34.67	35.17	35.50	35.03
	NCH ₃	38.13	37.92	34.42	37.03	38.26	38.43	38.76
Dimethylformamide	C	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH ₃	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH ₃	31.45	31.03	30.73	30.72	31.32	31.61	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	18.41	18.89	18.51	18.72	18.80	18.40	17.47
	CH ₂	58.28	57.72	56.07	57.86	57.96	58.26	58.05
Ethyl acetate	CH ₃ CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH ₂	60.49	60.56	59.74	60.21	60.98	61.50	62.32
	CH ₃	14.19	14.50	14.40	14.19	14.54	14.49	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	14.14	14.34	13.88	14.32	14.43	14.45	
	CH ₂ (2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH ₂ (3)	31.64	32.30	30.95	31.96	32.36	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	14.08	14.29	13.28	14.25	14.37	14.39	
	CH ₂ (2)	22.38	22.98	21.70	22.81	23.08	23.38	
	CH ₂ (3)	34.16	34.83	33.48	34.45	34.89	35.30	
2-Propanol	CH ₃	25.14	25.67	25.43	25.18	25.55	25.27	24.38
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
Pyridin	CH (2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH (3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH (4)	135.96	136.56	136.05	123.28	136.89	138.35	138.27
Silicone grease	CH ₃	1.04	1.40		1.38		2.10	
Tetrahydrofuran	CH ₂	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH ₂ O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
Toluene	CH ₃	21.46	21.46	20.99	21.10	21.50	21.50	
	CH (i)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH (o)	129.07	129.76	128.88	129.33	129.94	129.91	
	CH (m)	128.26	129.03	128.18	128.56	129.23	129.20	
	CH (p)	125.33	126.12	125.29	125.68	126.28	126.29	
Triethylamine	CH ₃	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH ₂	46.25	47.07	45.74	46.77	47.10	46.96	47.19
Xylenes								
o-Xylene	C (1,2)	136.49	137.03	135.91		137.51	137.37	
	CH (3,6)	129.59	130.28	129.29		130.46	130.47	
	CH (4,5)	125.79	126.58	125.61		126.78	126.81	
	CH ₃	19.71	19.68	19.24		19.79	19.77	
m-Xylene	C (1,3)	137.78	138.34	137.07		138.80	138.79	
	CH (2)	129.91	130.52	129.51		130.71	130.70	
	CH (5)	128.15	128.93	127.98		129.16	129.13	
	CH (4,6)	126.04	126.78	125.83		126.95	126.99	
	CH ₃	21.33	21.32	20.83		21.40	21.42	
p-Xylene	C (1,4)	134.67	135.27	134.03		135.68	135.71	
	CH (2,3,5,6)	128.92	129.65	128.69		129.85	129.84	
	CH ₃	20.94	20.94	20.49		21.00	21.02	