Electronic Supplementary Information for:

Development of GSK's NMR Guides – A tool to encourage the use of more sustainable solvents

Hugo E. Gottlieb,[a] Grazyna Graczyk-Millbrandt,[b] Graham G. A. Inglis,[c] Abraham Nudelman,[a] David Perez,[d] Yanqiu Qian,[b] Leanna E. Shuster,*[e] Helen F. Sneddon,[c] and Richard J. Upton.[c]

[a] *Department of Chemistry, Bar-Ilan University, Ramat-Gan 52900, Israel*

[b] *GSK, 709 Swedeland Road, King of Prussia, PA 19406, USA*

[c] *GSK, Medicines Research Centre, Gunnels Wood Road, Stevenage, Herts., UK, SG1 2NY.*

[d] *C2M Aurochs Industrie, 3 Impasse du lac, Z.I. de la Plaine, 31140 Aucamville, France*

[e] *GSK, 1250 South Collegeville Road, Collegeville, PA 19426, USA. Fax: 610-917-7393; Tel: 610-917-4489; E-mail: leanna.e.shuster@gsk.com*

Table of Contents:

Section 1:

Annotation	Explanation
*	This peak as recorded in this deuterated solvent appears with a different multiplicity than as indicated in the table. Some instances in D_2O or methanol-*d4* are due to lack of coupling to H-bonded protons. In a few cases this results from overlap of analyte peaks with the solvent or water signals.
+	Multiple peaks are overlapping to form a multiplet that cannot be fully resolved
R	The analyte and deuterated solvents are reactive with each other
N/O	This peak was not observed in the given spectrum.
a	For the ^{1}H NMR spectrum of glycerol in acetone-d_6, the shifts for all 6 carbon-bonded protons appear overlapped as a single, complex multiplet.
b	Peak assignments made on the basis of H-H COSY and HSQC 2D NMR spectra.
c	This peak is listed as a methylene group, but the two protons are non-equivalent, therefore this peak represents only a single proton.
d	Peak assignments made on the basis of H-H COSY, HSQC, HMQC, APT, and nOe 2D NMR spectra.
e	This peak represents 6 methylene protons from the cyclopentyl ring of CPME.
f	This peak represents 4 methylene protons from the cyclopentyl ring of CPME.
g	For dimethyl isosorbide in CD_3CN, one of the two protons which overlap in the other examined deuterated solvents to form the complex multiplet listed as "*CH*$_2$C(OMe) + *CH*(OMe)" on this table instead overlaps with the CH_2O multiplet at 3.76-3.80 ppm. In CD_3CN only, the peak at 3.76-3.80 therefore represents 2H, while the peak at 3.80-3.84 ppm represents 1H.
	Solvent is classified as amber by the GSK Solvent Sustainability Guide
	Solvent is classified as green by the GSK Solvent Sustainability Guide
Note: For data taken from literature references, most peaks labeled as multiplets reported a single chemical shift value and are therefore not shown here as a range, while those determined for this work are reported as a range, encompassing the full width of the signal.	

Table 1: Reference for all annotations and notes used in NMR chemical shift figures

Section 2:

NMR Shifts for Residual Solvent Impurities (^{1}H)

Solvent (bp)				D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
Acetic acid (118°C)		CH_3	**s**	2.08	1.91	1.96	1.96	1.99	2.10
Acetone (56°C)		CH_3	s	2.22	2.09	2.09	2.08	2.15	2.17
Acetonitrile (82°C)		CH_3	s	2.06	2.07	2.05	1.96	2.03	2.10
t-Amyl alcohol (102°C)		CH_3	t	0.89	0.82	0.89	0.87	0.91	0.92
		$(CH_3)_2$	s	1.19	1.05	1.13	1.11	1.15	1.20
		CH_2	q	1.51	1.35	1.45	1.43	1.48	1.51
		OH	s	N/O	4.02	3.06	2.25	N/O	1.29
t-Amyl methyl ether (85°C)		CH_3CH_2	t	0.85	0.79	0.83	0.83	0.86	0.87
		$(CH_3)_2C$	s	1.17	1.05	1.07	1.08	1.13	1.13
		CH_2	q	1.55	1.42	1.46	1.46	1.51	1.49
		CH_3O	s	3.20	3.05	3.10	3.10	3.17	3.18
Anisole (154°C)		CH_3	s	3.85	3.74	3.78	3.77	3.77	3.81
		CH(*o*/*p*)	m	7.01-7.10	6.89-6.97	6.88-6.95	6.89-6.98	6.85-6.95	6.87-6.98
		CH(*m*)	m	7.36-7.45	7.25-7.33	7.24-7.31	7.27-7.34	7.20-7.28	7.26-7.32
1-Butanol (118°C)		CH_3	t	0.91	0.87	0.90	0.91	0.93	0.94
		CH_2(3)	m	1.30-1.40	1.25-1.34	1.31-1.41	1.29-1.39	1.34-1.43	1.33-1.45
		CH_2(2)	m	1.49-1.56	1.35-1.43	1.44-1.52	1.42-1.49	1.47-1.55	1.52-1.59
		OH	t	--	4.30	3.35	2.44	--	--
		CH_2(1)	m	3.61	3.38	3.49-3.56	3.45-3.51	3.54	3.65
2-Butanol (100°C)		CH_3(4)	t	0.89	0.83	0.89	0.88	0.91	0.93
		CH_3(1)	d	1.16	1.02	1.09	1.08	1.13	1.19
		CH_2	m	1.43-1.52	1.25-1.40	1.33-1.47	1.33-1.42	1.36-1.52	1.42-1.54
		OH	d	--	4.29	3.33	2.47	--	1.40*
		CH	m	3.71-3.80	3.44-3.54	3.56-3.66	3.54-3.62	3.59-3.67	3.68-3.79
t-Butanol (82°C)		CH_3	s	1.24	1.11	1.18	1.16	1.40	1.28
		OH	s	--	4.19	--	2.18	--	--
n-Butyl acetate (126°C)		CH_3CH_2	t	0.91	0.89	0.92	0.92	0.94	0.94
		CH_2	m	1.31-1.43	1.27-1.37	1.32-1.43	1.31-1.42	1.33-1.45	1.34-1.43
		CH_2	m	1.59-1.68	1.50-1.58	1.54-1.62	1.54-1.63	1.55-1.65	1.57-1.65
		CH_3CO	s	2.09	1.99	1.97	1.97	2.01	2.04
		CH_2CO	t	4.12	3.99	4.02	4.02	4.06	4.07
t-Butyl acetate (95°C)		CH_3CO	s	1.46	1.39	1.41	1.42	1.44	1.45
		$(CH_3)_3C$	s	2.02	1.91	1.89	1.90	1.93	1.96
t-Butyl ethyl ether (70°C)		CH_3CH_2	t	1.15	1.04	1.06	1.07	1.13	1.16
		CCH_3	s	1.23	1.12	1.14	1.14	1.19	1.20
		CH_2	q	3.54	3.32	3.37	3.38	3.45	3.41
t-Butyl methyl ether (55°C)		CCH_3	s	1.21	1.11	1.13	1.14	1.15	1.19
		OCH_3	s	3.22	3.08	3.13	3.13	3.20	3.22
Butylene carbonate (250°C)		CH_3	t	0.98	0.91	0.99	0.96	R	1.04
		CH_2CH_3	m	1.74-1.88	1.70*	1.80	1.67-1.81	--	1.71-1.88
		CH_2O^1	dd	4.28	4.14	4.17	4.08	--	4.09
		CH_2O^1	t	4.67	4.55	4.61	4.51	--	4.53
		CHO	m	4.85-4.92	4.74	4.73-4.80	4.64-4.71	--	4.60*
Chloroform (61°C)		CH	s	insoluble	8.32	8.02	7.58	7.90	7.26
2,4,6-Collidine (171°C)		CH_3(*p*)	s	2.25	2.21	2.23	2.23	2.28	2.26
		CH_3(*m*)	s	2.39	2.36	2.37	2.38	2.43	2.47
		CH	s	6.91	6.85	6.82	6.83	6.91	6.78
Cyclohexane (81°C)		CH_2	s	insoluble	1.40	1.43	1.44	1.45	1.43
Cyclohexanone (155°C)		CH_2(4)	m	1.69-1.76	1.61-1.68	1.69-1.75	1.66-1.73	R	1.69-1.76
		CH_2(3)	m	1.83-1.91	1.73-1.79	1.78-1.85	1.78-1.85	--	1.83-1.90
		CH_2CO	t	2.39	2.25	2.27	2.27	--	2.34
Cyclopentyl methyl ether (106°C)		CH_2	m	1.52-1.68[e]	1.41-1.51	1.44-1.54	1.45-1.55	1.47-1.59	1.47-1.57
		CH_2	m	1.74-1.85	1.51-1.59[f]	1.55-1.71[e]	1.55-1.64[f]	1.60-1.68[f]	1.60-1.75[e]
		CH_2	m	--	1.59-1.67	--	1.64-1.73	1.69-1.76	--
		CH_3	s	3.30	3.15	3.19	3.20	3.26	3.28
		CH	m	3.94-3.99	3.69-3.77	3.72-3.77	3.73-3.80	3.80-3.86	3.77-3.82

NMR Shifts for Residual Solvent Impurities (^{1}H)

Solvent (bp)				D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
p-Cymene[b] (177°C)	CH_3CH	d	insoluble	1.17	1.20	1.20	1.21	1.23
	CH_3Ar	s	--	2.25	2.27	2.28	2.27	2.32
	$CH(CH_3)_2$	spt	--	2.83	2.85	2.85	2.83	2.87
	ArCH	m	--	7.05-7.15	7.06-7.13	7.06-7.15	7.02-7.10	7.11
1,2-Dichloroethane (84°C)	CH_2	s	insoluble	3.90	3.87	3.81	3.78	3.73
Dichloromethane (40°C)	CH_2	s	insoluble	5.76	5.63	5.44	5.49	5.30
Diethyl carbonate (127°C)	CH_3	t	1.28	1.20	1.24	1.24	1.26	1.31
	CH_2	q	4.21	4.10	4.13	4.12	4.14	4.19
Diethyl ether (35°C)	CH_3	t	1.17	1.09	1.11	1.12	1.18	1.21
	CH_2	q	3.56	3.38	3.41	3.42	3.49	3.48
Diethyl succinate (218°C)	CH_3	t	1.26	1.17	1.21	1.21	1.24	1.26
	CH_2O	s	2.69	2.53	2.57	2.54	2.59	2.62
	CH_2CH_2	q	4.18	4.05	4.09	4.09	4.12	4.15
Diglyme (162°C)	OCH_3	s	3.37	3.24	3.28	3.29	3.35	3.39
	CH_2	m	3.61	3.38	3.47	3.45	3.58	3.57
	CH_2	m	3.67	3.51	3.56	3.53	3.61	3.65
1,2-Dimethoxyethane (85°C)	CH_3	s	3.37	3.24	3.28	3.28	3.35	3.40
	CH_2	s	3.60	3.43	3.46	3.45	3.52	3.55
Dimethyl carbonate (90°C)	CH_3	s	3.80	3.69	3.72	3.72	3.74	3.79
Dimethyl isosorbide[d] (94°C)	CH_3	s	3.42	3.26	3.31	3.31	3.36	3.38
	CH_3	s	3.45	3.31	3.37	3.36	3.42	3.47
	$CH_2C(OMe)$[c]	m	3.53-3.58	3.37-3.42	3.44-3.49	3.41-3.46	3.49-3.54	3.56-3.64
	CH_2O[c]	m	3.86-3.91	3.69-3.75	3.76-3.83	3.76-3.80[f,g]	3.82-3.87	3.87*
	$CH_2C(OMe)$[c]+ $CH(OMe)$	m	4.00-4.09	3.76-3.81	3.76-3.83	3.80-3.84[g]	3.87-3.89	3.90-4.02
	CH_2O[c]			3.83	3.86		3.91	4.52
	$CH(OMe)$	m	4.13-4.19	3.84-3.89	3.88-3.91	3.84-3.91	3.93-3.99	4.62-4.67
	CH (junction)	d	4.67	4.42	4.43	4.43	4.49	3.90-4.02
	CH (junction)	m	4.78	4.53-4.57	4.57-4.61	4.54-4.58	4.61-4.65	3.90-4.02
	CH (junction)	m	4.78	4.53-4.57	4.57-4.61	4.54-4.58	4.61-4.65	3.90-4.02
Dimethylacetamide (165°C)	CH_3CO	s	2.08	1.96	1.97	1.97	2.07	2.09
	NCH_3	s	2.90	2.78	2.83	2.83	2.92	2.94
	NCH_3	s	3.06	2.94	3.00	2.96	3.31	3.02
Dimethylformamide (153°C)	CH_3	s	2.86	2.73	2.78	2.77	2.85	2.88
	CH_3	s	3.00	2.89	2.94	2.89	3.01	2.96
	CH	s	7.91	7.95	7.96	7.92	7.92	8.02
Dimethyl sulfoxide (189°C)	CH_3	s	2.71	2.54	2.52	2.50	2.65	2.62
Dimethylimidazolidinone (225°C)	CH_3	s	2.74	2.63	2.68	2.67	2.74	2.78
	CH_2	s	3.37	3.20	3.23	3.21	3.31	3.27
1,4-Dioxane (102°C)	CH_2	s	3.75	3.57	3.59	3.60	3.66	3.71
1,3-Dioxolane (75°C)	OCH_2O	s	3.93	3.77	3.80	3.80	3.83	3.88
	CH_2CH_2	s	4.90	4.78	4.79	4.80	4.83	4.91
Ethanol (78°C)	CH_3	t	1.17	1.06	1.12	1.12	1.19	1.25
	CH_2	q	3.65	3.44	3.57	3.54	3.60	3.72
	OH	s	N/O	4.63	3.39	2.47	N/O	1.32
Ethyl acetate (77°C)	CH_3CH_2	t	1.24	1.17	1.20	1.20	1.24	1.26
	CH_3CO	s	2.07	1.99	1.97	1.97	2.01	2.05
	CH_2	q	4.14	4.03	4.05	4.06	4.09	4.12
Ethyl lactate[b] (154°C)	CH_3CH_2	t	1.28	1.19	1.23	1.24	1.27	1.30
	CH_3CH	d	1.41	1.24	1.32	1.31	1.36	1.42
	OH	d	N/O	5.33	4.07	3.28	N/O	2.81
	CH_2	m	4.23*	4.04-4.16	4.11-4.17	4.09-4.22	4.18*	4.20-4.31
	CH	m	4.39*	4.04-4.16	4.17-4.24	4.09-4.22	4.21-4.25	4.20-4.31

NMR Shifts for Residual Solvent Impurities (^{1}H)

Solvent (bp)				D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
Ethyl propionate[b] (99°C)		CH_3CH_2CO	t	1.10	1.02	1.07	1.07	1.10	1.14
		CH_3CH_2O	t	1.26	1.18	1.20	1.20	1.24	1.26
		CH_2CO	q	2.39	2.29	2.28	2.28	2.31	2.32
		CH_2O	q	4.16	4.05	4.07	4.07	4.11	4.13
Ethylene carbonate (248°C)		CH_2	s	4.62	4.48	4.57	4.45	R	4.53
Ethylene glycol (197°C)		CH	s	3.65	3.34	3.28	3.51	3.59	3.76
Formic acid (101°C)		H	s	8.22	8.18	8.11	8.03	8.08	8.02
Furfural[b] (162°C)		*CH*CHO	dd	6.77	6.79	6.74	6.67	6.70	6.61
		*CH*C(CHO)	d	7.58	7.55	7.43	7.36	7.42	7.26
		CH*CH*O	s	7.92*	8.11	7.94	7.81	7.88	7.70
		C-*CH*O	s	9.50	9.62	9.67	9.60	9.60	9.67
Glycerol (290°C)[a]		CH_2	m	3.52-3.59	3.25-3.31	3.47-3.61	3.39-3.46	3.48-3.54	insoluble
		CH_2	m	3.62-3.68	3.33-3.39	3.47-3.61	3.46-3.53	3.55-3.61	--
		CH	m	3.75-3.82	3.43	3.47-3.61	3.53-3.60	3.62-3.68	--
		OH(1)	t	N/O	4.37	3.47-3.61	2.69	N/O	--
		OH(2)	d	N/O	4.44	3.64	2.93	N/O	--
Glycerol diacetate (190°C)		CH_3	s	2.12	2.02	2.01	2.01	R	2.09
		CH_2	s	4.34	4.19	4.24	4.21	--	4.27
Glycerol triacetate[b] (259°C)		CH_3	s	2.12	2.02	2.02	2.01	R	2.08
		CH_3	s	2.14	2.03	2.03	2.02	--	2.09
		CH_2	dd	4.31	4.13	4.17	4.14	--	4.16
		CH_2	dd	4.37	4.22	4.29	4.22	--	4.30
		CH	tt	5.32	5.15	5.22	5.19	--	5.22-5.28*
n-Heptane (98°C)		CH_3	t	insoluble	0.86	0.88	0.89	0.90	0.89
		CH_2	m	-	1.26	1.21-1.35	1.21-1.35	1.31	1.28
n-Hexane (69°C)		CH_3	t	insoluble	0.86	0.88	0.89	0.90	0.88
		CH_2	m	-	1.25	1.28	1.28	1.29	1.26
1-Hexanol (156°C)		CH_3	t	0.88	0.86	0.88	0.89	0.87-0.94	0.86-0.93
		CH_2(3-5)	m	1.24-1.39	1.19-1.32	1.24-1.39	1.22-1.38	1.26-1.40	1.24-1.44
		CH_2(2)	m	1.50-1.59	1.36-1.44	1.45-1.55	1.43-1.51	1.48-1.57	1.52-1.61
		CH_2(1)	m	3.60	3.35-3.40	3.37	3.44-3.50	3.53	3.64
		OH	m	N/O	4.31	3.49-3.56	2.43	N/O	1.24-1.44
Isoamyl acetate (142°C)		$(CH_3)_2$	d	0.91	0.88	0.91	0.91	0.93	0.92
		CH_2CH	m	1.55	1.46	1.50	1.49	1.52	1.52
		CH	m	1.69	1.64	1.69	1.69	1.67	1.64-1.74
		CH_3CO	s	2.09	1.99	1.97	1.97	2.01	2.04
		CH_2O	t	4.15	4.02	4.06	4.05	4.09	4.09
Isoamyl alcohol (131°C)		CH_3	d	0.90	0.85	0.89	0.89	0.91	0.92
		CH_2CH	m	1.44	1.31	1.39	1.37	1.42	1.47
		CH	m	1.61-1.71	1.65	1.72	1.67	1.64-1.77	1.66-1.78
		CH_2OH	td	3.64*	3.41	3.53-3.59*	3.51	3.58*	3.68
		OH	t	N/O	4.27	3.32	2.40	N/O	1.26
Isobutanol (108°C)		CH_3	d	0.88	0.82	0.87	0.86	0.90	0.92
		CH	m	1.70-1.80	1.60	1.68	1.66	1.70	1.77
		CH_2	m	3.38	3.11-3.19	3.26-3.34	3.25	3.30	3.41
		OH	t	N/O	4.39	3.45	2.52	N/O	1.31
Isooctane[b] (99°C)		$(CH_3)_3C$	s	insoluble	0.88	0.90	0.90	0.90	0.90
		$(CH_3)_2$CH	d	-	0.90	0.91	0.91	0.92	0.91
		CH_2	d	-	1.11	1.14	1.14	1.14	1.12
		CH	m	-	1.59-1.70	1.68	1.68	1.63-1.73	1.60-1.71
Isopropyl acetate (89°C)		$(CH_3)_2$CH	d	1.25	1.17	1.19	1.19	1.22	1.23
		CH_3CO	s	2.07	1.96	1.94	1.94	1.99	2.02
		CH	m	4.98	4.86	4.91	4.91	4.95	4.99

NMR Shifts for Residual Solvent Impurities (^{1}H)

Solvent (bp)				D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
(*R*)-(+)-Limonene[b] (176°C)		CH_2CH_2C=[c]	m	insoluble	1.34-1.45	1.40-1.51	1.40-1.50	1.42-1.53	1.42-1.52
		CH_3C=CH	s	-	1.61	1.62	1.63	1.63	1.65
		CH_3C=CH_2	s	-	1.70	1.72	1.73	1.72	1.73
		CH_2CH_2C=[c]	m	-	1.71-1.77	1.78	1.75-1.81	1.79	1.79
		CH_2CH=	m	-	1.80-1.95	1.83-1.99	1.84-1.99	1.84-1.99	1.86-1.99
		CH + CH_2C(Me)	m	-	1.95-2.08	1.99-2.13	2.00-2.12	2.00-2.14	2.00-2.15
		CH_2=	s	-	4.69	4.69	4.71	4.69	4.70
		CH=	br s	-	5.37	5.38	5.39	5.38	5.40
Methanesulfonic acid (167°C)		CH_3	s	2.80	5.70	3.00	2.98	2.98	R
Methanol (65°C)		CH_3	s	3.34	3.16	3.31	3.28	3.34	3.49
		OH	s	N/O	4.01	3.12	2.16	N/O	1.09
Methyl acetate (57°C)		CH_3CO	s	2.09	1.92	1.98	1.99	2.02	2.05
		OCH_3	s	3.68	3.61	3.59	3.60	3.64	3.67
Methyl ethyl ketone (80°C)		CH_3CH_2	t	1.26	0.91	0.96	0.96	1.01	1.06
		CH_3CO	s	2.19	2.07	2.07	2.06	2.12	2.14
		CH_2CH_3	q	3.18	2.43	2.45	2.43	2.50	2.46
Methyl isobutyl ketone[b] (117°C)		$(CH_3)_2CH$	d	0.90	0.85	0.88	0.88	0.85	0.92
		CH	m	2.08	2.00	2.02-2.11	2.02-2.08	2.00	2.13
		CH_3CO	s	2.21	2.05	2.06	2.05	2.05	2.12
		CH_2	d	2.43	2.28	2.31	2.29	2.28	2.30
Methylcyclohexane[b] (101°C)		CH_2CH[c] (ax.)	m	insoluble	0.80-0.90	0.87-0.93	0.88-0.94	0.82-0.94	0.82-0.93
		CH_3	d	-	0.84	0.84	0.86	0.87	0.86
		CH_2[c] (4)(ax.)	m	-	1.04-1.14	1.07-1.17	1.08-1.18	1.09-1.20	1.06-1.17
		CH_2[c] (3)(ax.)	m	-	1.14-1.25	1.24	1.25	1.26	1.17-1.28
		CH	m	-	1.32	1.34	1.30-1.39	1.31-1.39	1.33
		all equatorial H's	m	-	1.56-1.67	1.58-1.70	1.58-1.71	1.60-1.73	1.58-1.72
2-Methyltetrahydrofuran[b] (78°C)		CH_3	d	1.23	1.12	1.14	1.15	1.21	1.23
		CH_2CH(Me)[c]	m	1.43-1.52	1.26-1.36	1.30-1.39	1.31-1.40	1.38-1.47	1.36-1.46
		CH_2CH_2O	m	1.86-2.01	1.73-1.88	1.76-1.91	1.77-1.91	1.84-1.99	1.80-1.95
		CH_2CH(Me)[c]	m	2.02-2.11	1.89-1.97	1.92-2.00	1.92-2.00	1.99-2.07	1.95-2.03
		CH_2O[c]	m	3.70-3.77	3.52-3.59	3.55-3.63	3.60	3.66-3.73	3.71
		CH_2O[c]	m	3.84-3.91	3.71-3.78	3.76-3.82	3.79	3.82-3.90	3.86-3.92
		CH	m	3.99-4.07	3.79-3.87	3.82-3.88	3.82-3.89	3.90-3.99	3.92-3.98
Nitromethane (101°C)		CH_3	s	4.40	4.42	4.43	4.31	4.34	4.33
1-Octanol (196°C)		CH_3	t	0.83-0.90*	0.86	0.88	0.89	0.90	0.88
		CH_2(3-7)	m	1.23-1.38	1.19-1.32	1.23-1.39	1.22-1.36	1.23-1.40	1.22-1.39
		CH_2(2)	m	1.51-1.59	1.36-1.44	1.46-1.53	1.42-1.51	1.48-1.56	1.57
		CH_2(1)	m	3.60*	3.35-3.40	3.48-3.55	3.43-3.50	3.53*	3.60-3.68
		OH	t	N/O	4.31	3.37	2.45	N/O	1.22-1.39
n-Pentane (36°C)		CH_3	t	insoluble	0.86	0.88	0.89	0.90	0.88
		CH_2	m	-	1.27	1.27	1.29	1.29	1.27
1-Pentanol (137°C)		CH_3	t	0.89	0.86	0.89	0.90	0.92	0.91
		CH_2(3/4)	m	1.26-1.39	1.21-1.33	1.27-1.37	1.25-1.38	1.28-1.40	1.29-1.40
		CH_2(2)	m	1.50-1.62	1.37-1.45	1.45-1.55	1.43-1.52	1.48-1.57	1.52-1.62
		CH_2(1)	t	3.60	3.37	3.37	2.46	3.53	
		OH	t	N/O	4.31*	3.48-3.55	3.44-3.51	N/O	3.64
1,2-Propanediol (187°C)		CH_3	d	1.14	1.00	1.07	1.04	1.12	1.16
		OH	t	N/O	4.44	3.57	2.75	N/O	2.75-2.96 *
		OH	d	N/O	4.38	3.54	2.81	N/O	2.75-2.96*
		CH_2	m	3.41-3.47	3.12-3.19	3.30-3.37	3.21-3.30	3.40*	3.34-3.43
		CH_2	m	3.51-3.58	3.26*	3.37-3.44	3.34-3.42	3.41*	3.57-3.67
		CH	m	3.84-3.92	3.52-3.60	3.69-3.79	3.64-3.74	3.75	3.84-3.95
1,3-Propanediol (214°C)		CH_2(2)	quint	1.80	1.56	1.70	1.66	1.74	1.83*
		CH_2(1/3)	t	3.96	4.30	3.54	2.73	3.65	2.11*
		OH	m	N/O	3.39-3.51	3.62-3.70	3.55-3.65	N/O	3.81-3.91

NMR Shifts for Residual Solvent Impurities (^{1}H)

Solvent (bp)				D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
1-Propanol (97°C)		CH_3	t	0.90	0.83	0.89	0.88	0.92	0.94
		CH_2(2)	m	1.49-1.62	1.36-1.46	1.44-1.55	1.43-1.52	1.49-1.60	1.56*
		CH_2(1)	m	3.56*	3.33-3.37	3.44-3.51	3.40-3.47	3.5*	3.55-3.67
		OH	t	N/O	4.34	3.39	2.47	N/O	1.42*
2-Propanol (82°C)		CH_3	d	1.18	1.04	1.10	1.09	1.15	1.21
		CH	m	4.05	3.77	3.85-3.95	3.81-3.92	3.92	4.03
		OH	d	N/O	4.34	3.37	2.51	N/O	1.38
Propionic Acid (141°C)		CH_3	t	1.07	0.99	1.07	1.06	1.10	1.16
		CH_2	q	2.32	2.21	2.29	2.29	2.30	2.39
		OH	br s	N/O	11.95	N/O	8.85	N/O	N/O
n-Propyl acetate (102°C)		CH_3CH_2	t	0.92	0.88	0.92	0.92	0.94	0.94
		CH_2CH_3	m	1.65	1.57	1.61	1.61	1.64	1.65
		CH_3CO	s	2.09	2.00	1.98	1.98	2.02	2.05
		CH_2CO	t	4.06	3.95	3.97	3.97	4.01	4.02
Propylene carbonate (242°C)		CH_3	d	1.48	1.37	1.45	1.40	R	1.50
		CH_2	m	4.20*	4.03-4.10	4.05-4.13	3.95-4.07	--	4.03*
		CH_2	m	4.66-4.73	4.52-4.59	4.58-4.67	4.48-4.58	--	4.52-4.59
		CH	m	4.99-5.08	4.84-4.95	4.86-5.00	4.80-4.90	--	4.81-4.90
Pyridine (115°C)		CH(2)	m	8.52	8.58	8.58	8.57	8.53	8.62
		CH(3)	m	7.45	7.39	7.35	7.33	7.44	7.29
		CH(4)	m	7.87	7.79	7.76	7.73	7.85	7.68
Tetrahydrofuran (65°C)		CH_2	m	1.88	1.76	1.79	1.80	1.87	1.85
		CH_2O	m	3.74	3.60	3.63	3.64	3.71	3.76
Toluene (111°C)		CH_3	s	insoluble	2.30	2.32	2.33	2.32	2.36
		CH(*o*/*p*)	m	-	7.18	7.1-7.2	7.1-7.3	7.16	7.17
		CH(*m*)	m	-	7.25	7.1-7.2	7.1-7.3	7.16	7.25
Triethylamine (89°C)		CH_3	t	1.07	0.99	1.10	1.07	1.06	1.16
		CH_2	q	2.32	2.21	2.30	2.29	2.29	2.39
		OH	br s	N/O	11.95	N/O	N/O	8.85	N/O
Water (100°C)		H_2O	s	--	3.33	2.84	2.13	4.87	1.56
γ-Valerolactone[b] (207°C)		CH_3	d	1.41	1.30	1.34	1.34	R	1.42
		CH_2CH(Me)[c]	m	1.91	1.74	1.82	1.78	--	1.83
		CH_2CH(Me)[c]	m	2.37-2.47	2.23-2.32	2.33-2.41	2.26-2.37	--	2.36
		$CH_2C{=}O$	m	2.58-2.73	2.43-2.58	2.42-2.56	2.40-2.54	--	2.49-2.61
		CH	m	4.83	4.55-4.66	4.57-4.66	4.55-4.66	--	4.60-4.69
		CH	m	4.83	4.55-4.66	4.57-4.66	4.55-4.66	--	4.60-4.69
p-Xylene (138°C)		CH_3	s	2.30	2.24	2.26	2.27	2.26	2.30
		CH	s	7.18	7.05	7.04	7.06	7.02	7.06

Section 3:

NMR Shifts for Residual Solvent Impurities (^{13}C)

Solvent (bp)		D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
Acetic acid (118°C)	CH_3	21.03	20.95	20.51	20.73	20.56	20.81
	CO	177.21	171.93	172.31	173.21	175.11	175.99
Acetone (56°C)	CH_3	30.89	30.56	30.60	30.91	30.67	30.92
	CO	215.94	206.31	205.87	207.43	209.67	207.07
Acetonitrile (82°C)	CH_3	1.47	1.03	1.12	1.79	0.85	1.89
	CN	119.68	117.91	117.60	118.26	118.06	116.43
t-Amyl alcohol (102°C)	CH_3CH_2	10.72	8.53	8.90	8.97	8.95	8.60
	$(CH_3)_2$	30.01	28.65	29.13	29.04	28.64	28.69
	CH_2	38.09	35.84	37.06	37.08	37.12	36.38
	C	74.93	68.76	70.16	70.85	71.63	71.20
t-Amyl methyl ether (85°C)	CH_3CH_2	10.40	7.99	8.40	8.55	8.47	8.22
	$(CH_3)_2C$	26.49	24.18	24.73	24.83	24.83	24.49
	CH_2	33.91	31.57	32.88	32.88	32.97	32.10
	CH_3O	51.17	48.26	48.95	49.17	49.33	49.04
	C	80.06	73.82	74.72	75.18	76.50	74.79
Anisole (154°C)	CH_3	58.12	54.80	55.34	55.78	55.55	55.13
	C(*i*)	116.94	113.75	114.66	114.85	114.89	113.89
	CH(*o*)	124.19	120.33	121.25	121.53	121.59	120.65
	CH(*m*)	132.70	129.34	130.22	130.50	130.42	129.43
	CH(*p*)	189.21	159.11	160.68	160.74	161.16	159.55
1-Butanol (118°C)	CH_3	15.91	13.75	14.21	14.26	14.24	13.86
	CH_2(3)	21.22	18.54	19.73	19.81	20.03	18.90
	CH_2(2)	36.29	34.59	35.93	35.81	35.81	34.89
	CH_2(1)	64.41	60.27	62.13	62.35	62.69	62.76
2-Butanol (100°C)	CH_3CH_2	12.03	9.96	10.41	10.46	10.40	9.96
	CH_3CH	24.20	22.98	23.50	23.38	22.95	22.94
	CH_2	33.65	31.60	32.87	32.85	32.83	32.07
	CH	72.24	67.03	68.92	69.32	70.00	69.52
t-Butanol (82°C)	CH_3	30.29	30.38	30.72	30.68	30.91	31.25
	C	70.36	66.88	68.13	68.74	69.40	69.15
n-Butyl acetate (126°C)	CH_3CH_2	15.78	13.44	13.95	14.04	14.05	13.71
	CH_2	21.33	18.51	19.76	19.88	20.19	19.14
	CH_3CO	23.32	20.62	20.78	21.15	20.84	21.01
	CH_2	32.70	30.07	31.48	31.51	31.84	30.67
	CH_2	68.38	63.39	64.43	64.87	65.46	64.37
	CO	177.72	170.3	170.95	171.78	173.09	171.25
t-Butyl acetate (95°C)	CH_3CO	24.90	22.10	22.32	22.67	22.41	22.54
	$(CH_3)_3C$	30.06	27.65	28.21	28.30	28.33	28.09
	C	85.33	79.37	80.06	80.59	81.54	80.16
	CO	176.88	169.62	170.39	171.16	172.56	170.56
t-Butyl methyl ether (55°C)	CCH_3	26.60	26.79	27.24	27.28	27.22	26.99
	OCH_3	49.37	48.70	49.35	49.52	49.66	49.45
	C	75.62	72.04	72.81	73.17	74.32	72.87
t-Butyl ethyl ether (72°C)	CH_3CH_2	17.83	16.09	16.65	16.73	16.47	16.33
	$(CH_3)_3$	29.35	27.30	27.85	27.90	27.86	27.62
	CH_2	60.19	55.91	57.06	57.35	58.03	56.77
	$C(CH_3)_3$	77.68	71.80	72.58	72.98	74.26	72.57
Butylene carbonate (250°C)	CH_3	10.42	8.23	8.79	8.85	R	8.52
	CH_2O	28.83	25.86	27.35	27.37	--	26.99
	CH_2CH_3	72.94	68.73	69.76	70.15	--	69.00
	CH	82.73	77.84	78.83	79.28	--	77.98
	CO	160.89	154.82	155.69	156.39	--	155.06
Chloroform (61°C)	CH	insoluble	79.16	79.19	79.17	79.44	77.36

NMR Shifts for Residual Solvent Impurities (^{13}C)

Solvent (bp)		D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
2,4,6-Collidine (171°C)	$CH_3(p)$	22.84	20.16	20.65	20.82	20.83	20.78
	$CH_3(o)$	25.20	23.69	24.27	24.36	23.49	24.29
	CH	124.62	120.75	121.51	121.83	122.84	121.18
	$\boldsymbol{C}CH_3(p)$	152.95	146.84	147.93	148.59	150.47	147.44
	$\boldsymbol{C}CH_3(o)$	159.70	156.63	158.04	158.35	158.26	157.39
Cyclohexane (81°C)	CH_2	insoluble	26.33	27.51	27.63	27.96	26.94
Cyclohexanone (155°C)	$CH_2(4)$	26.98	24.22	25.62	25.67	R	25.02
	$CH_2(3)$	29.71	26.35	27.71	27.86	--	27.03
	$CH_2(2)$	44.24	41.23	42.27	42.50	--	42.00
	CO	223.50	210.67	210.27	212.11	--	212.12
Cyclopentyl methyl ether (106°C)	CH_2CH_2O	25.87	23.04	24.14	24.29	24.45	23.55
	CH_2O	34.13	31.33	32.51	32.64	32.85	31.97
	CH_3	58.29	55.44	56.18	56.40	56.54	56.34
	CH	86.68	81.89	83.33	83.61	84.48	82.98
p-Cymene[b] (177°C)	CH_3Ar	insoluble	20.47	20.94	21.00	21.04	20.96
	$(\boldsymbol{C}H_3)_2CH$	--	23.89	24.39	24.42	24.56	24.11
	$CH(CH_3)_2$	--	32.89	34.36	34.47	34.97	33.69
	CH	--	125.97	126.94	127.23	127.18	126.27
	CH	--	128.70	129.66	129.90	129.89	128.97
	$\boldsymbol{C}CH$	--	134.44	135.64	136.16	136.15	135.14
	$\boldsymbol{C}CH_3$	--	145.19	146.47	146.90	146.98	145.88
1,2-Dichloroethane (84°C)	CH_2	insoluble	45.02	45.25	45.54	45.11	43.50
Dichloromethane (40°C)	CH_2	insoluble	54.84	54.95	55.32	54.78	53.52
Diethyl carbonate (127°C)	CH_3	16.29	14.01	14.55	14.60	14.61	14.29
	CH_2	67.71	63.19	64.03	64.50	64.76	63.78
	CO	158.83	154.41	155.86	156.09	156.79	155.18
Diethyl ether (35°C)	CH_3	14.77	15.12	15.78	15.63	15.46	15.20
	CH_2	66.42	62.05	66.12	66.32	66.88	65.91
Diethyl succinate (218°C)	CH_3	16.14	13.96	14.49	14.57	14.51	14.19
	CH_2CH_2	31.96	28.53	29.68	29.88	30.03	29.22
	CH_2O	64.80	59.89	60.80	61.29	61.75	60.68
	CO	178.09	171.78	172.65	173.28	174.17	172.33
Diglyme (162°C)	CH_3	58.67	57.98	58.77	58.90	59.06	59.01
	CH_2	70.05	69.54	71.03	70.99	71.33	70.51
	CH_2	71.63	71.25	72.63	72.63	72.92	71.90
1,2-Dimethoxyethane (85°C)	CH_3	58.67	58.01	58.45	58.89	59.06	59.08
	CH_2	71.49	17.07	72.47	72.47	72.72	71.84
Dimethyl carbonate (90°C)	CH_3	58.06	54.56	54.96	55.41	55.30	54.85
	CO	160.04	155.63	157.05	157.29	157.99	156.40
Dimethyl isosorbide (94°C)	OCH_3	59.47	56.16	56.90	57.23	57.32	57.17
	OCH_3	60.53	57.08	57.86	58.18	58.44	58.23
	CH_2	72.05	69.19	70.72	70.62	71.00	69.77
	CH_2	75.39	72.00	73.27	73.54	73.94	73.04
	CH (junction)	82.54	79.37	80.87	80.94	81.51	79.92
	CH(OMe)	83.71	80.92	82.54	82.61	83.00	81.80
	CH (junction)	87.70	85.03	86.71	86.68	87.03	85.91
	CH(OMe)	87.81	85.05	86.81	86.81	87.07	85.93
Dimethylacetamide (165°C)	CH_3	21.09	21.29	21.51	21.76	21.32	21.53
	NCH_3	35.03	37.38	34.89	35.17	35.50	35.28
	NCH_3	38.76	34.42	37.92	38.26	38.43	38.13
	CO	174.57	169.54	170.61	171.31	173.32	171.07
Dimethylformamide (153°C)	CH_3	32.03	30.73	31.03	31.32	31.61	31.45
	CH_3	37.54	35.73	36.15	36.57	36.89	36.50
	CH	165.53	162.29	162.79	163.31	164.73	162.62
Dimethyl sulfoxide (189°C)	CH_3	39.39	40.45	41.23	41.31	40.45	40.76

NMR Shifts for Residual Solvent Impurities (^{13}C)

Solvent (bp)		D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
Dimethylimidazolidinone (225°C)	CH_3	33.68	31.08	31.65	31.85	31.56	31.53
	CH_2	47.88	44.37	45.62	45.81	46.13	45.09
	CO	166.86	161.27	162.37	163.00	164.19	162.10
1,4-Dioxane (102°C)	CH_2	67.19	66.36	67.60	67.72	68.11	67.14
1,3-Dioxolane (75°C)	CH_2CH_2	67.09	63.74	65.00	65.21	65.51	64.58
	OCH_2O	96.94	93.98	95.34	95.57	95.84	95.09
Ethanol (78°C)	CH_3	17.47	18.51	18.89	18.80	18.40	18.41
	CH_2	58.05	56.07	57.72	57.96	58.26	58.28
Ethyl acetate (77°C)	CH_3	13.92	14.40	14.50	14.54	14.49	14.19
	CH_3CO	21.15	20.68	20.83	21.16	20.88	21.04
	CH_2	62.32	59.74	60.56	60.98	61.50	60.49
	CO	175.26	170.31	170.96	171.68	172.89	171.36
Ethyl lactate[b] (154°C)	CH_3CH_2	16.14	14.01	14.48	14.55	14.53	14.19
	CH_3CH	22.01	20.28	20.78	20.80	20.59	20.42
	CH_2	65.13	59.85	61.16	61.78	62.00	61.69
	CH	69.61	65.82	67.42	67.61	67.91	66.76
	CO	179.43	174.45	175.57	176.01	176.43	175.75
Ethyl propionate (99°C)	CH_3CH_2CO	11.22	8.89	9.38	9.49	9.46	9.14
	CH_3CH_2O	16.17	14.02	14.54	14.62	14.54	14.26
	CH_2CO	30.32	26.71	27.82	28.12	28.38	27.64
	CH_2O	64.45	59.57	60.43	60.90	61.44	60.24
	CO	180.91	173.49	174.29	175.10	176.30	174.53
Ethylene carbonate (248°C)	CH_2	68.88	64.89	65.69	66.04	R	64.59
	CO	161.38	155.44	156.28	156.98	--	155.41
Ethylene glycol (197°C)	CH_2	63.17	62.76	64.26	64.22	64.30	63.79
Formic acid (101°C)	CO_2H	165.19	162.98	162.32	162.72	164.42	165.02
Furfural (162°C)	CHCHO	116.12	112.81	113.44	113.66	113.81	112.58
	CHC(CHO)	153.05	122.90	122.25	123.06	123.27	120.93
	CHCHO	183.57	149.10	149.33	149.66	150.14	148.06
	C	154.96	152.41	154.21	154.13	154.58	153.02
	C-CHO	218.56	178.31	178.43	179.07	179.69	177.88
Glycerol (290°C)	CH_2	65.35	62.97	64.57	64.37	64.47	insoluble
	CH	74.92	72.37	73.37	73.29	73.91	--
Glycerol diacetate (190°C)	CH_3	23.10	20.50	20.65	21.01	R	20.81
	CH_2	65.68	61.81	62.81	63.06	--	62.19
	CO	176.98	170.14	170.87	171.56	--	170.78
Glycerol triacetate (259°C)	CH_3CO	22.96	20.38	20.55	20.90	R	20.69
	CH_3CO	23.18	20.57	20.78	21.11	--	20.89
	CH_2	65.58	61.82	62.85	63.07	--	62.27
	CH	72.60	68.73	69.96	70.00	--	69.08
	CO	176.12	169.68	170.43	171.07	--	170.12
	CO	176.67	169.98	170.70	171.40	--	170.51
n-Heptane (98°C)	CH_3	insoluble	13.90	14.33	14.43	14.45	14.12
	CH_2	--	22.05	23.32	23.45	23.77	22.71
	CH_2	--	28.32	29.74	29.81	30.19	29.03
	CH_2	--	31.21	32.60	32.67	33.08	31.90
n-Hexane (69°C)	CH_3	insoluble	13.88	14.34	14.43	14.45	14.14
	CH_2 (2)	--	22.05	23.28	23.40	23.68	22.70
	CH_2 (3)	--	30.95	32.30	32.36	32.73	31.64
1-Hexanol (156°C)	CH_3	16.17	13.84	14.32	14.39	14.40	14.03
	CH_2(5)	24.80	22.06	23.35	23.45	23.74	22.65
	CH_2(4)	27.58	25.08	26.37	26.38	26.67	25.44
	CH_2(3)	33.69	31.11	32.51	32.51	32.90	31.66
	CH_2(2)	34.11	32.42	33.77	33.65	33.67	32.79
	CH_2(1)	64.76	60.63	62.49	62.68	63.05	63.09

NMR Shifts for Residual Solvent Impurities (^{13}C)

Solvent (bp)		D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
Isoamyl acetate (142°C)	CH_3CH	23.34	20.64	20.80	21.17	20.86	21.03
	$(CH_3)_2$	24.49	22.19	22.70	22.75	22.82	22.46
	CH	27.24	24.41	25.75	25.89	26.27	25.08
	CH_2CH	39.36	36.77	38.16	38.17	38.53	37.34
	CH_3O	67.20	62.14	63.19	63.64	64.20	63.16
	C=O	N/O	170.27	170.93	171.75	173.05	171.23
Isoamyl alcohol (131°C)	CH_3	24.63	22.51	22.98	22.96	23.03	22.62
	CH	26.87	24.13	25.42	25.55	25.86	24.72
	$CH_2(2)$	43.17	41.50	42.80	42.65	42.71	41.76
	$CH_2(1)$	63.03	58.86	60.70	60.93	61.27	61.37
Isobutanol (108°C)	CH_3	21.05	19.01	19.37	19.32	19.40	18.86
	CH	32.60	30.37	31.74	31.74	31.96	30.85
	CH_2	71.50	67.64	69.44	69.52	69.95	69.81
Isooctane[b] (99°C)	CH	insoluble	24.04	25.28	25.40	25.79	24.61
	$(CH_3)_3C$	--	25.24	25.77	25.80	25.92	25.48
	$(CH_3)_2CH$	--	29.83	30.35	30.37	30.55	30.10
	C	--	30.69	31.51	31.59	31.84	31.05
	CH_2	--	52.55	53.79	53.84	54.34	53.09
Isopropyl acetate (89°C)	CH_3CO	insoluble	21.06	21.21	21.57	21.25	21.44
	$(CH_3)_2CH$	--	21.56	22.00	22.07	22.00	21.84
	CH	--	66.93	67.75	68.26	69.07	67.64
	CO	--	169.78	170.41	171.21	172.54	170.66
(*R*)-(+)-Limonene[b] (176°C)	$CH_3C=CH_2$	insoluble	20.55	20.93	21.03	21.00	20.83
	$CH_3C=CH$	--	23.16	23.60	23.65	23.65	23.48
	$CH_2CH_2C=$	--	27.25	28.68	28.84	29.19	27.94
	$CH_2C=^c$	--	29.91	31.10	31.18	31.54	30.61
	$CH_2C=^c$	--	30.05	31.48	31.59	31.92	30.83
	CH	--	40.27	41.89	41.98	42.52	41.11
	$CH_2=$	--	108.62	108.90	108.98	108.98	108.36
	CH=	--	120.31	121.32	121.50	121.61	120.65
	C	--	132.96	134.09	134.58	134.57	133.76
	C	--	149.27	150.72	151.37	151.21	150.29
Methanesulfonic acid (167°C)	CH_3	41.42	39.52	39.72	39.98	39.47	R
Methanol (65°C)	CH_3	49.50	48.59	49.77	49.90	49.86	50.41
Methyl acetate (57°C)	CH_3CO	20.55	20.45	20.47	20.84	20.48	20.67
	CH_3O	52.59	51.21	51.54	52.02	52.06	51.58
	CO	175.54	170.80	171.34	172.16	173.36	171.51
Methyl cyclohexane[b] (101°C)	CH_3	insoluble	22.65	23.17	23.25	23.32	22.91
	$CH_2(4)$	--	25.67	26.94	27.10	27.43	26.35
	$CH_2(3)$	--	25.73	27.07	27.22	27.56	26.46
	CH	--	32.01	33.45	33.57	34.03	32.74
	$CH_2(2)$	--	34.77	36.09	36.19	36.61	35.45
Methyl ethyl ketone (80°C)	CH_3CH_2	7.87	7.61	8.03	8.14	8.09	7.86
	CH_3CO	29.49	29.26	29.30	29.60	29.39	29.49
	CH_2CH_3	37.27	35.83	36.75	37.09	37.34	36.89
	CO	218.43	208.72	208.30	209.88	212.16	209.56
Methyl isobutyl ketone (117°C)	$(CH_3)_2$	19.62	22.28	22.72	22.76	22.80	22.53
	CH	22.52	23.85	25.03	25.29	25.68	24.63
	CH_3CO	27.62	30.03	30.15	30.44	30.26	30.34
	CH_2	50.36	51.76	52.78	53.04	53.38	52.80
	CO	215.72	208.16	207.71	209.44	211.81	208.97

NMR Shifts for Residual Solvent Impurities (^{13}C)

Solvent (bp)		D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
2-Methyl tetrahydrofuran (78°C)	CH_3	22.58	20.81	21.26	21.33	21.12	20.97
	$CH_2(4)$	28.03	25.32	26.43	26.58	26.76	25.91
	$CH_2(3)$	35.17	32.61	33.75	33.83	34.04	33.10
	$CH_2(5)$	70.39	66.64	67.93	68.10	68.68	67.73
	CH	79.09	74.20	75.49	75.78	76.75	75.23
1-Octanol (196°C)	CH_3	insoluble	13.85	14.35	14.43	14.45	14.10
	$CH_2(7)$	--	21.99	23.32	23.44	23.75	22.66
	$CH_2(6)$	--	25.41	26.71	26.71	26.99	25.76
	$CH_2(5)$	--	28.65	30.10	30.13	30.47	29.28
	$CH_2(4)$	--	28.82	30.25	30.25	30.61	29.41
	$CH_2(3)$	--	31.16	32.61	32.65	33.04	31.82
	$CH_2(2)$	--	32.45	33.81	33.68	33.71	32.83
	$CH_2(1)$	--	60.62	62.49	62.68	63.05	63.11
Nitromethane (101°C)	CH_3	63.22	63.28	63.21	63.66	63.08	62.50
n-Pentane (36°C)	CH_3	insoluble	13.28	14.29	14.37	14.39	14.08
	CH_2 (2)	--	21.70	22.98	23.08	23.38	22.38
	CH_2 (3)	--	33.48	34.83	34.89	35.30	34.16
1-Pentanol (137°C)	CH_3	16.16	13.91	14.37	14.43	14.42	14.04
	$CH_2(4)$	24.63	21.93	23.23	23.30	23.60	22.50
	$CH_2(3)$	30.17	27.64	28.90	28.91	29.21	27.93
	$CH_2(2)$	33.83	32.12	33.48	33.37	33.39	32.51
	$CH_2(1)$	64.73	60.61	62.47	62.65	63.02	63.07
1,2-Propanediol (187°C)	CH_3	20.82	19.87	19.76	19.53	19.56	18.79
	CH	69.44	67.08	68.64	68.49	68.62	68.03
	CH_2	70.77	67.14	68.66	68.75	69.25	68.34
1,3-Propanediol (214°C)	$CH_2(2)$	36.62	35.70	36.40	36.09	36.32	34.08
	$CH_2(1/3)$	61.47	57.87	60.44	60.56	60.06	62.22
1-Propanol (97°C)	CH_3	12.42	10.33	10.66	10.68	10.62	10.15
	$CH_2(2)$	27.45	25.53	26.77	26.74	26.71	25.91
	$CH_2(1)$	66.43	62.37	64.19	64.36	64.73	64.69
2-Propanol (82°C)	CH_3	26.56	25.38	25.79	25.67	25.29	25.38
	CH	67.11	61.91	63.72	64.15	64.78	64.44
Propionic Acid (141°C)	CH_3	11.90	8.99	9.39	9.39	9.53	8.83
	CH_2	31.32	26.80	27.37	27.52	28.15	27.39
	CO_2H	184.54	175.07	175.36	176.19	178.35	180.69
n-Propyl acetate (102°C)	CH_3CH_2	8.09	10.20	10.59	10.65	10.66	10.37
	CH_2O	19.00	20.66	22.69	22.79	20.81	21.00
	CH_3CO	19.83	21.46	20.75	21.13	23.04	21.97
	CH_2CH_3	65.82	65.23	66.20	66.60	67.23	66.10
	CO	173.44	170.37	170.96	171.78	173.10	171.26
Propylene carbonate (242°C)	CH_3	21.09	18.72	19.36	19.42	R	19.47
	CH_2	74.54	70.37	71.40	71.76	--	70.64
	CH	78.46	73.66	74.45	74.94	--	73.49
	CO	160.80	154.78	155.66	156.36	--	154.98
Pyridine (115°C)	CH(3)	125.12	123.84	124.57	127.76	125.53	123.75
	CH(4)	138.27	136.05	136.56	136.89	138.35	135.96
	CH(2)	149.18	149.58	150.67	150.76	150.07	149.90

NMR Shifts for Residual Solvent Impurities (^{13}C)

Solvent (bp)		D_2O	$(CD_3)_2SO$	$(CD_3)_2CO$	CD_3CN	CD_3OD	$CDCl_3$
Tetrahydrofuran (65°C)	CH_2	25.67	25.14	26.15	26.27	26.48	25.62
	CH_2O	68.68	67.03	68.07	68.33	68.83	67.97
Toluene (111°C)	CH_3	insoluble	20.99	21.46	21.50	21.50	21.46
	CH(*p*)	--	125.29	126.12	126.28	126.29	125.33
	CH(*m*)	--	128.18	129.03	129.23	129.20	128.26
	CH(*o*)	--	128.88	129.76	129.94	129.91	129.07
	C(*i*)	--	137.35	138.48	138.90	138.85	137.89
Triethylamine (89°C)	CH_3	9.07	11.74	12.49	12.38	11.09	11.61
	CH_2	47.19	45.74	47.07	47.10	46.96	46.25
γ-Valerolactone[b] (207°C)	CH_3	22.80	20.64	21.21	21.23	R	21.09
	CH_2C=O	31.75	28.50	29.37	29.69	--	29.09
	CH_2CH(Me)	31.97	28.98	29.69	30.28	--	29.73
	CH	82.98	76.62	77.46	78.18	--	77.24
	CO	185.24	177.02	177.21	178.35	--	177.19
p-Xylene (138°C)	CH_3	22.79	20.47	20.94	21.02	21.03	20.95
	CH	131.92	128.66	129.65	129.87	129.84	128.90
	C	188.56	133.98	135.24	135.70	135.71	134.67