

Supporting Information

NMR Chemical Shifts of Trace Impurities: Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist

Gregory R. Fulmer,^{*,1} Alexander J. M. Miller,² Nathaniel H. Sherden,² Hugo E.
Gottlieb,³ Abraham Nudelman,³ Brian M. Stoltz,² John E. Bercaw,² and Karen I.
Goldberg¹

¹ *Department of Chemistry, University of Washington, Box 351700, Seattle, Washington 98195-1700;*

² *Arnold and Mabel Beckman Laboratories of Chemical Synthesis, and Caltech Center for Catalysis and
Chemical Synthesis, Division of Chemistry and Chemical Engineering California Institute of Technology,
Pasadena, California 91125;*

³ *Department of Chemistry, Bar Ilan University, Ramat Gan 52900, Israel.*

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Corrections and Comments

In the preparation of this manuscript, several errors were discovered in the original paper¹ and are reported herein. While comparing the ¹H NMR spectral data obtained in toluene-*d*₈ to that in C₆D₆, it was discovered that the ¹H NMR chemical shifts for acetic acid (CH₃), acetonitrile (CH₃) and *tert*-butyl alcohol (OH) in C₆D₆ had each been misreported at 1.55 ppm in the original paper; the values have now been correctly listed as 1.52, 0.58, and 0.63 ppm, respectively. The original paper's assignments for BHT's C(3,5) and C(4) in C₆D₆, (CD₃)₂CO, (CD₃)₂SO, CD₃CN, and CD₃OD were reversed and are now corrected. The resonances for 1,2-dimethoxyethane (CH₂) in (CD₃)₂CO, silicone grease (CH₃) in CDCl₃, and 2-propanol (CH₃) in CD₃OD have been corrected and are reported as 72.47, 1.04, and 1.15 ppm, respectively. No other significant differences were discovered when comparing our data to that which had been previously reported; however, we have additionally provided the OH resonance for ethanol in C₆D₆ (0.50 ppm), the CH₃ resonance for silicone grease in (CD₃)₂SO (−0.06 ppm), and replaced the “grease” entry (formerly motor oil¹) with VWR vacuum pump oil #19, which is now reported in each deuterated solvent.

<i>n</i> -hexane	CH ₃	t, 7	0.89	0.89	0.88	0.88	0.89	0.85	0.88	0.86	0.89	0.91	0.90	-
	CH ₂	m	1.29	1.27	1.26	1.22	1.24	1.19	1.28	1.25	1.28	1.31	1.29	-
HMPA	CH ₃	d, 9.5	2.58	2.60	2.65	2.42	2.40	2.47	2.59	2.53	2.57	2.63	2.64	2.61
hydrogen	H ₂	s	4.55	4.59	4.62	4.50	4.47	4.49	4.54	4.61	4.57	4.53	4.56	-
imidazole	CH(2)	s	7.48	7.63	7.67	7.30	7.33	7.53	7.62	7.63	7.57	7.61	7.67	7.78
	CH(4,5)	s	6.94	7.07	7.10	6.86	6.90	7.01	7.04	7.01	7.01	7.03	7.05	7.14
methane	CH ₄	s	0.19	0.21	0.22	0.17	0.16	0.15	0.17	0.20	0.20	0.18	0.20	0.18
methanol	CH ₃	s ⁹	3.27	3.42	3.49	3.03	3.07	3.25	3.31	3.16	3.28	3.44	3.34	3.34
	OH	s ^{5,9}	3.02	1.09	1.09	-	-	1.30	3.12	4.01	2.16	-	-	-
nitromethane	CH ₃	s	4.31	4.31	4.33	3.01	2.94	3.59	4.43	4.42	4.31	4.28	4.34	4.40
<i>n</i> -pentane	CH ₃	t, 7	0.89	0.89	0.88	0.87	0.87	0.84	0.88	0.86	0.89	0.90	0.90	-
	CH ₂	m	1.31	1.30	1.27	1.25	1.23	1.23	1.27	1.27	1.29	1.33	1.29	-
propane	CH ₃	t, 7.3	0.90	0.90	0.90	0.89	0.86	0.84	0.88	0.87	0.90	0.90	0.91	0.88
	CH ₂	sept, 7.3	1.33	1.32	1.32	1.32	1.26	1.26	1.31	1.29	1.33	1.33	1.34	1.30
2-propanol	CH ₃	d, 6	1.08	1.17	1.22	0.95	0.95	1.04	1.10	1.04	1.09	1.20	1.15	1.17
	CH	sept, 6	3.82	3.97	4.04	3.65	3.67	3.82	3.90	3.78	3.87	4.05	3.92	4.02
propylene	CH ₃	dt, 6.4, 1.5	1.69	1.71	1.73	1.55	1.55	1.58	1.68	1.68	1.70	1.70	1.70	1.70
	CH ₂ (1)	dm, 10	4.89	4.93	4.94	4.92	4.95	4.91	4.90	4.94	4.93	4.93	4.91	4.95
	CH ₂ (2)	dm, 17	4.99	5.03	5.03	4.98	5.01	4.98	5.00	5.03	5.04	5.03	5.01	5.06
	CH	m	5.79	5.84	5.83	5.70	5.72	5.72	5.81	5.80	5.85	5.87	5.82	5.90
pump oil	CH ₃	m	0.86–0.90	0.84–0.89	0.83–0.89	0.88–0.96	0.91–0.97	0.88–0.91	0.87	0.74	0.85	0.99	0.86–0.91	-
	CH ₂	br s	1.29	1.27	1.26	1.30	1.37	1.31	1.29	1.15	1.27	1.41	1.29	-
pyridine	CH(2,6)	m	8.54	8.59	8.62	8.47	8.53	8.51	8.58	8.58	8.57	8.45	8.53	8.52
	CH(3,5)	m	7.25	7.28	7.29	6.67	6.66	6.90	7.35	7.39	7.33	7.40	7.44	7.45
	CH(4)	m	7.65	7.68	7.68	6.99	6.98	7.25	7.76	7.79	7.73	7.82	7.85	7.87
pyrrole	NH	br t	9.96	8.69	8.40	7.71	7.80	8.61	10.02	10.75	9.27	-	-	-
	CH(2,5)	m	6.66	6.79	6.83	6.43	6.48	6.62	6.77	6.73	6.75	6.84	6.72	6.93
	CH(3,4)	m	6.02	6.19	6.26	6.27	6.37	6.27	6.07	6.01	6.10	6.24	6.08	6.26
pyrrolidine ¹⁰	CH ₂ (2,5)	m	2.75	2.82	2.87	2.54	2.54	2.64	-	2.67	2.75	3.11	2.80	3.07
	CH ₂ (3,4)	m	1.59	1.67	1.68	1.36	1.33	1.43	-	1.55	1.61	1.93	1.72	1.87
silicone grease	CH ₃	s	0.11	0.09	0.07	0.26	0.29	0.14	0.13	-0.06	0.08	0.16	0.10	-
tetrahydrofuran	CH ₂ (2,5)	m	3.62	3.69	3.76	3.54	3.57	3.59	3.63	3.60	3.64	3.78	3.71	3.74
	CH ₂ (3,4)	m	1.79	1.82	1.85	1.43	1.40	1.55	1.79	1.76	1.80	1.91	1.87	1.88
toluene	CH ₃	s	2.31	2.34	2.36	2.11	2.11	2.16	2.32	2.30	2.33	2.33	2.32	-
	CH(2,4,6)	m	7.10	7.15	7.17	6.96–7.01	7.02	7.01–7.08	7.10–7.20	7.18	7.10–7.30	7.10–7.30	7.16	-
	CH(3,5)	m	7.19	7.24	7.25	7.09	7.13	7.10–7.17	7.10–7.20	7.25	7.10–7.30	7.10–7.30	7.16	-
triethylamine	CH ₃	t, 7	0.97	0.99	1.03	0.95	0.96	0.93	0.96	0.93	0.96	1.31	1.05	0.99
	CH ₂	q, 7	2.46	2.48	2.53	2.39	2.40	2.39	2.45	2.43	2.45	3.12	2.58	2.57

ethyl acetate	$C H_3CO$	20.45	21.15	21.04	20.46	20.56	20.50	20.83	20.68	21.16	21.18	20.88	21.15
	CO	170.32	171.24	171.36	170.02	170.44	170.20	170.96	170.31	171.68	175.55	172.89	175.26
	CH_2	60.30	60.63	60.49	60.08	60.21	60.06	60.56	59.74	60.98	62.70	61.50	62.32
	CH_3	14.37	14.37	14.19	14.23	14.19	14.07	14.50	14.40	14.54	14.36	14.49	13.92
ethyl methyl ketone	$C H_3CO$	28.92	29.55	29.49	28.74	28.56	28.82	29.30	29.26	29.60	29.64	29.39	29.49
	CO	207.05	209.57	209.56	206.31	206.55	206.87	208.30	208.72	209.88	218.31	212.16	218.43
	$C H_2CH_3$	36.59	37.01	36.89	36.32	36.36	36.39	36.75	35.83	37.09	38.23	37.34	37.27
	$CH_2C H_3$	7.87	7.94	7.86	7.89	7.91	7.79	8.03	7.61	8.14	8.29	8.09	7.87
ethylene	CH_2	123.09	123.20	123.13	122.92	122.96	122.95	123.47	123.52	123.69	124.08	123.46	-
ethylene glycol	CH_2	64.35	64.08	63.79	64.29	64.34	64.03	64.26	62.76	64.22	64.87	64.30	63.17
furan	$CH(2,5)$	143.26	142.98	142.71	142.65	142.73	142.49	143.49	142.82	143.74	144.22	143.68	143.57
	$CH(3,4)$	109.88	109.86	109.57	109.63	109.67	109.64	110.24	109.62	110.49	111.06	110.33	110.23
H grease ⁸	CH_2	30.45	30.14	29.71	30.31	30.22	30.11	-	-	-	-	-	-
hexamethylbenzene	C	131.88	132.09	132.21	131.72	131.79	131.54	132.22	131.10	132.61	134.04	132.53	-
	CH_3	16.71	16.93	16.98	16.84	16.95	16.68	16.86	16.60	16.94	17.04	16.90	-
hexamethyldisiloxane	CH_3	1.83	1.96	1.97	1.99	2.05	1.92	2.01	1.96	2.07	2.09	1.99	2.31
<i>n</i> -hexane	CH_3	14.22	14.28	14.14	14.34	14.32	14.18	14.34	13.88	14.43	14.63	14.45	-
	$CH_2(2,5)$	23.33	23.07	22.70	23.12	23.04	22.86	23.28	22.05	23.40	24.06	23.68	-
	$CH_2(3,4)$	32.34	32.01	31.64	32.06	31.96	31.77	32.30	30.95	32.36	33.17	32.73	-
HMPA ¹¹	CH_3	36.89	36.99	36.87	36.80	36.88	36.64	37.04	36.42	37.10	37.21	37.00	36.46
imidazole	$CH(2)$	135.72	135.76	135.38	135.57	135.76	135.50	135.89	135.15	136.33	136.58	136.31	136.65
	$CH(4,5)$	122.20	122.16	122.00	122.13	122.16	121.96	122.31	121.55	122.78	122.93	122.60	122.43
methane	CH_4	-4.90	-4.33	-4.63	-4.34	-4.29	-4.33	-5.33	-4.01	-4.61	-5.88	-4.90	-
methanol	CH_3	49.64	50.45	50.41	49.90	49.97	49.66	49.77	48.59	49.90	50.67	49.86	49.50 ¹²
nitromethane	CH_3	62.49	63.03	62.50	61.14	61.16	61.68	63.21	63.28	63.66	63.17	63.08	63.22
<i>n</i> -pentane	CH_3	14.18	14.24	14.08	14.27	14.25	14.10	14.29	13.28	14.37	14.54	14.39	-
	$CH_2(2,4)$	23.00	22.77	22.38	22.79	22.72	22.54	22.98	21.70	23.08	23.75	23.38	-
	$CH_2(3)$	34.87	34.57	34.16	34.54	34.45	34.26	34.83	33.48	34.89	35.76	35.30	-
propane	CH_3	16.60	16.63	16.63	16.65	16.66	16.56	16.68	16.34	16.73	16.93	16.80	-
	CH_2	16.82	16.63	16.37	16.63	16.60	16.48	16.78	15.67	16.91	17.46	17.19	-
2-propanol	CH_3	25.70	25.43	25.14	25.24	25.18	25.14	25.67	25.43	25.55	25.21	25.27	24.38
	CH	66.14	64.67	64.50	64.12	64.23	64.18	63.85	64.92	64.30	66.69	64.71	64.88
propylene	CH_3	19.27	19.47	19.50	19.32	19.38	19.32	19.42	19.20	19.48	19.63	19.50	-
	CH_2	115.74	115.70	115.74	115.89	115.92	115.86	116.03	116.07	116.12	116.38	116.04	-
	CH	134.02	134.21	133.91	133.61	133.69	133.57	134.34	133.55	134.78	136.00	134.61	-
pump oil	CH_2	30.63	30.13	29.84	30.33	30.24	30.11	30.36	29.33	30.86	31.85	31.35	-
pyridine	$CH(2,6)$	150.57	150.27	149.90	150.25	150.27	149.93	150.67	149.58	150.76	149.76	150.07	149.18
	$CH(3,5)$	124.08	124.06	123.75	123.46	123.58	123.49	124.57	123.84	127.76	126.27	125.53	125.12
	$CH(4)$	135.99	136.16	135.96	135.17	135.28	135.32	136.56	136.05	136.89	139.62	138.35	138.27
pyrrole	$CH(2,5)$	118.03	117.93	117.77	117.61	117.78	117.65	117.98	117.32	118.47	119.61	118.28	119.06
	$CH(3,4)$	107.74	108.02	107.98	108.15	108.21	108.03	108.04	107.07	108.31	108.85	108.11	107.83
pyrrolidine ¹⁰	$CH_2(2,5)$	45.82	47.02	46.93	47.12	46.86	46.75	-	46.51	47.57	47.43	47.23	46.83
	$CH_2(3,4)$	26.17	25.83	25.56	25.75	25.65	25.59	-	25.26	26.34	25.73	26.29	25.86
silicone grease	CH_3	1.20	1.22	1.19	1.37	1.38	1.09	1.40	-	-	2.87	2.10	-
tetrahydrofuran	$CH_2(2,5)$	68.03	68.16	67.97	67.75	67.80	67.64	68.07	67.03	68.33	69.53	68.83	68.68
	$CH_2(3,4)$	26.19	25.98	25.62	25.79	25.72	25.68	26.15	25.14	26.27	26.69	26.48	25.67
toluene	CH_3	21.29	21.53	21.46	21.37	21.10	21.23	21.46	20.99	21.50	21.62	21.50	-
	C(1)	138.24	138.36	137.89	137.84	137.91	137.65	138.48	137.35	138.90	139.92	138.85	-
	$CH(2,6)$	129.47	129.35	129.07	129.33	129.33	129.12	129.76	128.88	129.94	130.58	129.91	-
	$CH(3,5)$	128.71	128.54	128.26	128.51	128.56	128.31	129.03	128.18	129.23	129.79	129.20	-
triethylamine	$CH(4)$	125.84	125.62	125.33	125.66	125.68	125.43	126.12	125.29	126.28	126.82	126.29	-
	CH_3	12.51	12.12	11.61	12.39	12.35	11.87	12.49	11.74	12.38	9.51	11.09	9.07
	CH_2	47.18	46.75	46.25	46.82	46.77	46.36	47.07	45.74	47.10	48.45	46.96	47.19

Table S3. THF- d_8 (^1H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.07	s	CH ₃	hexamethyldisiloxane	2.21	s	ArCH ₃	BHT	4.50	ddd	CH ₂	allyl acetate
0.11	s	CH ₃	silicone grease	2.24	t	CH ₂ (2,6)	cyclohexanone	4.55	s	H ₂	hydrogen
0.19	s	CH ₄	methane	2.31	s	CH ₃	toluene	4.58	ddd	CH ₂	diallyl carbonate
0.85	s	CH ₃	ethane	2.39	q, 7	CH ₂ CH ₃	ethyl methyl ketone	4.89	dm, 10	CH ₂ (1)	propylene
0.85-0.91	m	CH ₃	H grease ⁸	2.45	s	CH ₃	dimethyl sulfoxide	4.99	dm, 17	CH ₂ (2)	propylene
0.86-0.90	m	CH ₃	pump oil	2.46	s	OH	water	5.15	ddt	CHCH ₂ (2)	allyl acetate
0.89	t, 7	CH ₃	<i>n</i> -hexane	2.46	q, 7	CH ₂	triethylamine	5.19	ddt	CHCH ₂ (2)	diallyl carbonate
0.89	t, 7	CH ₃	<i>n</i> -pentane	2.58	d, 9.5	CH ₃	HMPA	5.27	ddt	CHCH ₂ (1)	allyl acetate
0.90	t, 7.3	CH ₃	propane	2.75	m	CH ₂ (2,5)	pyrrolidine	5.31	ddt	CHCH ₂ (1)	diallyl carbonate
0.96	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.76	s	CH ₃	dimethylformamide	5.36	s	CH ₂	ethylene
0.97	t, 7	CH ₃	triethylamine	2.82	s	NCH ₃	dimethylacetamide	5.51	s	CH ₂	dichloromethane
1.08	d, 6	CH ₃	2-propanol	2.88	s	CH ₃	dimethylformamide	5.64	s	OH	BHA
1.10	t, 7	CH ₃	ethanol	2.95	s	NCH ₃	dimethylacetamide	5.79	m	CH	propylene
1.12	t, 7	CH ₃	diethyl ether	3.02	s ^o	OH	methanol	5.81	s	OH	BHT
1.15	s	CH ₃	<i>tert</i> -butyl alcohol	3.16	s	OH	<i>tert</i> -butyl alcohol	5.90	ddt	CHCH ₂	allyl acetate
1.19	t, 7	CH ₂ CH ₃	ethyl acetate	3.27	s ^o	CH ₃	methanol	5.92	ddt	CHCH ₂	diallyl carbonate
1.29	br s	CH ₂	H grease ⁸	3.28	s	OCH ₃	diglyme	6.02	m	CH(3,4)	pyrrole
1.29	m	CH ₂	<i>n</i> -hexane	3.28	s	CH ₃	1,2-dimethoxyethane	6.37	dd	CH(3,4)	furan
1.29	br s	CH ₂	pump oil	3.30	s ^o	OH	ethanol	6.66	m	CH(2,5)	pyrrole
1.31	m	CH ₂	<i>n</i> -pentane	3.35	s	CH ₂	dimethyl malonate	6.68	s	ArH	BHA
1.33	sept, 7.3	CH ₂	propane	3.38	q, 7	CH ₂	diethyl ether	6.92	s	ArH	BHT
1.40	s	ArC(CH ₃) ₃	BHA	3.43	m	CH ₂	diglyme	6.94	s	CH(4,5)	imidazole
1.40	s	ArC(CH ₃) ₃	BHT	3.43	s	CH ₂	1,2-dimethoxyethane	7.10	m	CH(2,4,6)	toluene
1.44	s	CH ₂	cyclohexane	3.48	s	CH ₂	ethylene glycol	7.19	m	CH(3,5)	toluene
1.59	m	CH ₂ (3,4)	pyrrolidine	3.51	q, 7 ^o	CH ₂	ethanol	7.25	m	CH(3,5)	pyridine
1.68-1.71	m	CH ₂ (4)	cyclohexanone	3.53	m	CH ₂	diglyme	7.31	s	CH	benzene
1.69	dt, 6.4, 1.5	CH ₃	propylene	3.56	s	CH ₂	1,4-dioxane	7.48	dd	CH(2,5)	furan
1.72	m	CHD(3,4)	THF- d_8 residual	3.57	s	CH ₂	18-crown-6	7.48	s	CH(2)	imidazole
1.77-1.82	m	CH ₂ (3,5)	cyclohexanone	3.58	m	CHD(2,5)	THF- d_8 residual	7.51-7.55	m	CH(3,5)	benzaldehyde
1.79	m	CH ₂ (3,4)	tetrahydrofuran	3.62	m	CH ₂ (2,5)	tetrahydrofuran	7.60-7.64	m	CH(4)	benzaldehyde
1.89	s	CH ₃	acetic acid	3.65	s	CH ₃	dimethyl malonate	7.65	m	CH(4)	pyridine
1.94	s	CH ₂ CO	dimethylacetamide	3.68	s	ArOCH ₃	BHA	7.86-7.88	m	CH(2,6)	benzaldehyde
1.94	s	CH ₂ CO	ethyl acetate	3.69	s	CH ₃	dimethyl carbonate	7.89	s	CH	chloroform
1.95	s	CH ₃	acetonitrile	3.77	s	CH ₂	1,2-dichloroethane	7.91	s	CH	dimethylformamide
1.98	s	CH ₃	allyl acetate	3.82	sept, 6	CH	2-propanol	8.54	m	CH(2,6)	pyridine
2.03	s	CH ₂ CO	ethyl methyl ketone	4.04	q, 7	CH ₂ CH ₃	ethyl acetate	9.96	br t	NH	pyrrole
2.05	s	CH ₃	acetone	4.31	s	CH ₃	nitromethane	9.98	s	HCO	benzaldehyde
2.18	s	CH ₃	hexamethylbenzene								

Table S4. THF- d_8 ($^{13}\text{C}\{^1\text{H}\}$ NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.90	CH ₄	methane	30.17	CH ₃	acetone	64.35	CH ₂	ethylene glycol	129.47	CH(2,6)	toluene
0.45	CH ₃	acetonitrile	30.45	CH ₂	H grease ⁸	65.31	CH ₂	allyl acetate	129.56	CH(3,5)	benzaldehyde
1.20	CH ₂	silicone grease	30.57	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	66.14	CH ₂	diethyl ether	129.98	CH(2,6)	benzaldehyde
1.83	CH ₃	hexamethyldisiloxane	30.63	CH ₂	pump oil	66.14	CH	2-propanol	131.88	C	hexamethylbenzene
6.79	CH ₃	ethane	30.65	(CH ₃) ₃ C	BHA	67.21 (p)	CD ₂ (2,5)	THF- d_8 signal	133.08	CHCH ₂	diallyl carbonate
7.87	CH ₂ CH ₃	ethyl methyl ketone	30.70	CH ₃	dimethylformamide	67.50	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	133.90	CHCH ₂	allyl acetate
12.51	CH ₃	triethylamine	31.55	(CH ₃) ₃ C	BHT	67.65	CH ₂	1,4-dioxane	134.02	CH	propylene
14.18	CH ₃	<i>n</i> -pentane	32.34	CH ₂ (3,4)	<i>n</i> -hexane	68.03	CH ₂ (2,5)	tetrahydrofuran	134.67	CH(4)	benzaldehyde
14.22	CH ₃	<i>n</i> -hexane	34.60	NCH ₃	dimethylacetamide	68.58	CH ₂	diallyl carbonate	135.72	CH(2)	imidazole
14.37	CH ₂	ethyl acetate	34.87	CH ₂ (3)	<i>n</i> -pentane	71.17	CH ₂	diglyme	135.99	CH(4)	pyridine
15.49	CH ₃	diethyl ether	34.91	(CH ₃) ₃ C	BHT	71.34	CH ₂	18-crown-6	137.78	C(1)	benzaldehyde
16.60	CH ₃	propane	35.51	(CH ₃) ₃ C	BHA	72.58	CH ₂	1,2-dimethoxyethane	137.93	C(2,6)	BHT
16.71	CH ₃	hexamethylbenzene	35.65	CH ₃	dimethylformamide	72.72	CH ₂	diglyme	138.24	C(1)	toluene
16.82	CH ₂	propane	36.59	CH ₂ CH ₃	ethyl methyl ketone	79.24	CH	chloroform	140.07	C(4)	BHA
18.90	CH ₃	ethanol	36.89 (d)	CH ₃	HMPA ¹¹	96.89	CCl ₄	carbon tetrachloride	143.26	CH(2,5)	furan
19.27	CH ₃	propylene	37.56	NCH ₃	dimethylacetamide	107.74	CH(3,4)	pyrrole	148.62	C(2,6)	BHA
20.13	CH ₂	acetic acid	41.15	CH ₂	dimethyl malonate	109.88	CH(3,4)	furan	150.57	CH(2,6)	pyridine
20.45	CH ₃	allyl acetate	41.21	CH ₃	dimethyl sulfoxide	110.94	CH(3,5)	BHA	152.48	C(1)	BHT
20.45	CH ₂ CO	ethyl acetate	42.17	CH ₂ (2,6)	cyclohexanone	115.74	CH ₂	propylene	154.07	C(1)	BHA
21.15	CH ₃	dimethylacetamide	44.64	CH ₂	1,2-dichloroethane	116.79	CN	acetonitrile	155.36	CO	diallyl carbonate
21.21	CH ₂ Ar	BHT	45.82	CH ₂ (2,5)	pyrrolidine	117.58	CHCH ₂	allyl acetate	156.91	CO	dimethyl carbonate
21.29	CH ₃	toluene	47.18	CH ₂	triethylamine	117.70	CHCH ₂	diallyl carbonate	161.96	CH	dimethylformamide
23.00	CH ₂ (2,4)	<i>n</i> -pentane	49.64	CH ₃	methanol	118.03	CH(2,5)	pyrrole	167.14	CO ₂	dimethyl malonate
23.33	CH ₂ (2,5)	<i>n</i> -hexane	52.07	CH ₃	dimethyl malonate	122.20	CH(4,5)	imidazole	169.77	CO	dimethylacetamide
25.31 (p)	CD ₂ (3,4)	THF- d_8 signal	54.58	CH ₃	dimethyl carbonate	123.09	CH ₂	ethylene	170.14	CO	allyl acetate
25.70	CH ₃	2-propanol	54.67	CH ₂	dichloromethane	124.08	CH(3,5)	pyridine	170.32	CO	ethyl acetate
25.76	CH ₂ (4)	cyclohexanone	55.39	CH ₂ O	BHA	125.69	CO ₂	carbon dioxide	171.69	CO	acetic acid
26.17	CH ₂ (3,4)	pyrrolidine	57.60	CH ₂	ethanol	125.71	CH(3,5)	BHT	191.95	HCO	benzaldehyde
26.19	CH ₂ (3,4)	tetrahydrofuran	58.72	CH ₃	diglyme	125.84	CH(4)	toluene	193.37	CS ₂	carbon disulfide
27.58	CH ₂	cyclohexane	58.72	CH ₃	1,2-dimethoxyethane	128.64	C(4)	BHT	204.19	CO	acetone
27.69	CH ₂ (3,5)	cyclohexanone	60.30	CH ₂	ethyl acetate	128.71	CH(3,5)	toluene	207.05	CO	ethyl methyl ketone
28.92	CH ₂ CO	ethyl methyl ketone	62.49	CH ₃	nitromethane	128.84	CH	benzene	208.79	CO	cyclohexanone

Table S5. CD₂Cl₂ (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.07	s	CH ₃	hexamethyldisiloxane	2.09	s	CH ₃ CO	ethyl methyl ketone	4.61	ddd	CH ₂	diallyl carbonate
0.09	s	CH ₃	silicone grease	2.12	s	CH ₃	acetone	4.76	s	OH	BHA
0.21	s	CH ₄	methane	2.20	s	CH ₃	hexamethylbenzene	4.93	dm, 10	CH ₂ (1)	propylene
0.84-0.89	m	CH ₃	pump oil	2.25	s	ArCH ₃	BHT	5.00	s	OH	BHT
0.84-0.90	m	CH ₃	H grease ⁸	2.29	t	CH ₂ (2,6)	cyclohexanone	5.03	dm, 17	CH ₂ (2)	propylene
0.85	s	CH ₃	ethane	2.34	s	CH ₃	toluene	5.22	ddt	CHCH ₂ (2)	allyl acetate
0.89	t, 7	CH ₃	n-hexane	2.43	q, 7	CH ₂ CH ₃	ethyl methyl ketone	5.26	ddt	CHCH ₂ (2)	diallyl carbonate
0.89	t, 7	CH ₃	n-pentane	2.48	q, 7	CH ₂	triethylamine	5.31	ddt	CHCH ₂ (1)	allyl acetate
0.90	t, 7,3	CH ₃	propane	2.55	s	CH ₃	dimethyl sulfoxide	5.32	t	CDHCl ₂	CD ₂ Cl ₂ residual
0.99	t, 7	CH ₃	triethylamine	2.60	d, 9,5	CH ₃	HMPA	5.33	s	CH ₂	dichloromethane
1.00	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.82	s	CH ₃	dimethylformamide	5.35	ddt	CHCH ₂ (1)	diallyl carbonate
1.09	s ⁹	OH	methanol	2.82	m	CH ₂ (2,5)	pyrrolidine	5.40	s	CH ₂	ethylene
1.15	t, 7	CH ₃	diethyl ether	2.87	s	NCH ₃	dimethylacetamide	5.84	m	CH	propylene
1.17	d, 6	CH ₃	2-propanol	2.91	s	CH ₃	dimethylformamide	5.92	ddt	CHCH ₂	allyl acetate
1.19	t, 7	CH ₃	ethanol	2.97	s	NCH ₃	dimethylacetamide	5.95	ddt	CHCH ₂	diallyl carbonate
1.23	t, 7	CH ₂ CH ₃	ethyl acetate	3.33	s	OCH ₃	diglyme	6.19	m	CH(3,4)	pyrrole
1.24	s	CH ₃	tert-butyl alcohol	3.34	s	CH ₃	1,2-dimethoxyethane	6.41	dd	CH(3,4)	furan
1.27	br s	CH ₂	H grease ⁸	3.37	s	CH ₂	dimethyl malonate	6.73	s	ArH	BHA
1.27	m	CH ₂	n-hexane	3.42	s ⁹	CH ₃	methanol	6.79	m	CH(2,5)	pyrrole
1.27	br s	CH ₂	pump oil	3.43	q, 7	CH ₂	diethyl ether	6.97	s	ArH	BHT
1.30	m	CH ₂	n-pentane	3.49	s	CH ₂	1,2-dimethoxyethane	7.07	s	CH(4,5)	imidazole
1.32	sept, 7,3	CH ₂	propane	3.50	m	CH ₂	diglyme	7.15	m	CH(2,4,6)	toluene
1.33	s ⁹	OH	ethanol	3.57	m	CH ₂	diglyme	7.24	m	CH(3,5)	toluene
1.42	s	ArC(CH ₃) ₃	BHA	3.59	s	CH ₂	18-crown-6	7.28	m	CH(3,5)	pyridine
1.42	s	ArC(CH ₃) ₃	BHT	3.65	s	CH ₂	1,4-dioxane	7.32	s	CH	chloroform
1.44	s	CH ₂	cyclohexane	3.66	q, 7 ⁹	CH ₂	ethanol	7.35	s	CH	benzene
1.52	s	OH	water	3.66	s	CH ₂	ethylene glycol	7.46	dd	CH(2,5)	furan
1.69-1.72	m	CH ₂ (4)	cyclohexanone	3.69	m	CH ₂ (2,5)	tetrahydrofuran	7.53-7.57	m	CH(3,5)	benzaldehyde
1.67	m	CH ₂ (3,4)	pyrrolidine	3.72	s	CH ₃	dimethyl malonate	7.63	s	CH(2)	imidazole
1.71	dt, 6,4, 1,5	CH ₃	propylene	3.73	s	ArOCH ₃	BHA	7.63-7.67	m	CH(4)	benzaldehyde
1.81-1.87	m	CH ₂ (3,5)	cyclohexanone	3.75	s	CH ₃	dimethyl carbonate	7.68	m	CH(4)	pyridine
1.82	m	CH ₂ (3,4)	tetrahydrofuran	3.76	s	CH ₂	1,2-dichloroethane	7.87-7.89	m	CH(2,6)	benzaldehyde
1.97	s	CH ₃	acetonitrile	3.97	sept, 6	CH	2-propanol	7.96	s	CH	dimethylformamide
2.00	s	CH ₂ CO	ethyl acetate	4.08	q, 7	CH ₂ CH ₃	ethyl acetate	8.59	m	CH(2,6)	pyridine
2.02	s	CH ₂ CO	dimethylacetamide	4.31	s	CH ₃	nitromethane	8.69	br t	NH	pyrrole
2.05	s	CH ₃	allyl acetate	4.55	ddd	CH ₂	allyl acetate	10.01	s	HCO	benzaldehyde
2.06	s	CH ₃	acetic acid	4.59	s	H ₂	hydrogen				

Table S6. CD₂Cl₂ (¹³C{¹H}) NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.33	CH ₄	methane	30.14	CH ₂	H grease ⁸	64.08	CH ₂	ethylene glycol	129.42	CH(3,5)	benzaldehyde
1.22	CH ₃	silicone grease	30.37	(CH ₃) ₃ C	BHA	64.67	CH	2-propanol	129.98	CH(2,6)	benzaldehyde
1.96	CH ₃	hexamethyldisiloxane	30.54	(CH ₃) ₃ C	BHT	65.36	CH ₂	allyl acetate	132.09	C	hexamethylbenzene
2.03	CH ₃	acetonitrile	31.00	CH ₃	acetone	66.11	CH ₂	diethyl ether	132.24	CHCH ₂	diallyl carbonate
6.91	CH ₃	ethane	31.39	CH ₃	dimethylformamide	67.47	CH ₂	1,4-dioxane	132.94	CHCH ₂	allyl acetate
7.94	CH ₂ CH ₃	ethyl methyl ketone	31.46	(CH ₃) ₃ C	tert-butyl alcohol	68.16	CH ₂ (2,5)	tetrahydrofuran	134.21	CH	propylene
12.12	CH ₃	triethylamine	32.01	CH ₂ (3,4)	n-hexane	68.76	CH ₂	diallyl carbonate	134.79	CH(4)	benzaldehyde
14.24	CH ₃	n-pentane	34.56	(CH ₃) ₃ C	BHT	69.11	(CH ₃) ₃ C	tert-butyl alcohol	135.76	CH(2)	imidazole
14.28	CH ₃	n-hexane	34.57	CH ₂ (3)	n-pentane	70.47	CH ₂	18-crown-6	136.16	CH(4)	pyridine
14.37	CH ₃	ethyl acetate	34.91	(CH ₃) ₃ C	BHA	70.70	CH ₂	diglyme	136.32	C(2,6)	BHT
15.44	CH ₃	diethyl ether	35.23	NCH ₃	dimethylacetamide	72.24	CH ₂	1,2-dimethoxyethane	136.98	C(1)	benzaldehyde
16.63	CH ₃	propane	36.56	CH ₃	dimethylformamide	72.25	CH ₂	diglyme	137.77	C(4)	BHA
16.63	CH ₂	propane	36.99 (d)	CH ₃	HMPA'	77.99	CH	chloroform	138.36	C(1)	toluene
16.93	CH ₃	hexamethylbenzene	37.01	CH ₂ CH ₃	ethyl methyl ketone	96.52	CCl ₄	carbon tetrachloride	142.98	CH(2,5)	furan
18.69	CH ₃	ethanol	38.22	NCH ₃	dimethylacetamide	108.02	CH(3,4)	pyrrole	148.06	C(2,6)	BHA
19.47	CH ₃	propylene	41.33	CH ₃	dimethyl sulfoxide	109.86	CH(3,4)	furan	150.27	CH(2,6)	pyridine
20.91	CH ₃	acetic acid	41.48	CH ₂	dimethyl malonate	110.93	CH(3,5)	BHA	151.92	C(1)	BHT
21.06	CH ₃	allyl acetate	42.31	CH ₂ (2,6)	cyclohexanone	115.7	CH ₂	propylene	153.05	C(1)	BHA
21.15	CH ₃ CO	ethyl acetate	44.35	CH ₂	1,2-dichloroethane	116.92	CN	acetonitrile	155.15	CO	diallyl carbonate
21.27	CH ₂ Ar	BHT	46.75	CH ₂	triethylamine	117.93	CH(2,5)	pyrrole	156.73	CO	dimethyl carbonate
21.53	CH ₃	toluene	47.02	CH ₂ (2,5)	pyrrolidine	118.00	CHCH ₂	allyl acetate	162.57	CH	dimethylformamide
21.64	CH ₃	dimethylacetamide	50.45	CH ₃	methanol	118.75	CHCH ₂	diallyl carbonate	167.32	CO ₂	dimethyl malonate
22.77	CH ₂ (2,4)	n-pentane	52.75	CH ₃	dimethyl malonate	122.16	CH(4,5)	imidazole	170.83	CO	allyl acetate
23.07	CH ₂ (2,5)	n-hexane	53.84 (p)	CD ₂ Cl ₂	CD ₂ Cl ₂ signal	123.20	CH ₂	ethylene	171.05	CO	dimethylacetamide
25.42	CH ₂ (4)	cyclohexanone	54.24	CH ₂	dichloromethane	124.06	CH(3,5)	pyridine	171.24	CO	ethyl acetate
25.43	CH ₃	2-propanol	55.09	CH ₃	dimethyl carbonate	125.26	CO ₂	carbon dioxide	175.85	CO	acetic acid
25.83	CH ₂ (3,4)	pyrrolidine	55.88	CH ₃ O	BHA	125.62	CH(4)	toluene	192.61	HCO	benzaldehyde
25.98	CH ₂ (3,4)	tetrahydrofuran	58.57	CH ₂	ethanol	125.84	CH(3,5)	BHT	192.95	CS ₂	carbon disulfide
27.38	CH ₂	cyclohexane	58.95	CH ₃	diglyme	128.54	CH(3,5)	toluene	206.78	CO	acetone
27.47	CH ₂ (3,5)	cyclohexanone	59.02	CH ₃	1,2-dimethoxyethane	128.68	CH	benzene	209.57	CO	ethyl methyl ketone
29.55	CH ₂ CO	ethyl methyl ketone	60.63	CH ₂	ethyl acetate	128.73	C(4)	BHT	211.82	CO	cyclohexanone
30.13	CH ₂	pump oil	63.03	CH ₃	nitromethane	129.35	CH(2,6)	toluene			

Table S7. CDCl₃ (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.07	s	CH ₃	hexamethyldisiloxane	2.14	s	CH ₃ CO	ethyl methyl ketone	4.64	ddd	CH ₂	diallyl carbonate
0.07	s	CH ₃	silicone grease	2.17	s	CH ₃	acetone	4.76	s	OH ^d	BHA
0.22	s	CH ₄	methane	2.24	s	CH ₃	hexamethylbenzene	4.94	dm, 10	CH ₂ (1)	propylene
0.83–0.89	m	CH ₃	pump oil	2.27	s	ArCH ₃	BHT	5.01	s	OH ^d	BHT
0.84–0.87	m	CH ₃	H grease ⁸	2.33	t	CH ₂ (2,6)	cyclohexanone	5.03	dm, 17	CH ₂ (2)	propylene
0.87	s	CH ₃	ethane	2.36	s	CH ₃	toluene	5.24	ddt	CHCH ₂ (2)	allyl acetate
0.88	t, 7	CH ₃	<i>n</i> -hexane	2.46	q, 7	CH ₂ CH ₃	ethyl methyl ketone	5.27	ddt	CHCH ₂ (2)	diallyl carbonate
0.88	t, 7	CH ₃	<i>n</i> -pentane	2.53	q, 7	CH ₂	triethylamine	5.30	s	CH ₂	dichloromethane
0.90	t, 7,3	CH ₃	propane	2.62	s	CH ₃	dimethyl sulfoxide	5.32	ddt	CHCH ₂ (1)	allyl acetate
1.03	t, 7	CH ₃	triethylamine	2.65	d, 9.5	CH ₃	HMPA	5.37	ddt	CHCH ₂ (1)	diallyl carbonate
1.06	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.87	m	CH ₂ (2,5)	pyrrolidine	5.40	s	CH ₂	ethylene
1.09	s ⁹	OH	methanol	2.88	s	CH ₃	dimethylformamide	5.83	m	CH	propylene
1.21	t, 7	CH ₃	diethyl ether	2.94	s	NCH ₃	dimethylacetamide	5.93	ddt	CHCH ₂	allyl acetate
1.22	d, 6	CH ₃	2-propanol	2.96	s	CH ₃	dimethylformamide	5.94	ddt	CHCH ₂	diallyl carbonate
1.25	t, 7	CH ₃	ethanol	3.02	s	NCH ₃	dimethylacetamide	6.26	m	CH(3,4)	pyrrole
1.25	br s	CH ₂	H grease ⁸	3.39	s	OCH ₃	diglyme	6.40	dd	CH(3,4)	furan
1.26	t, 7	CH ₂ CH ₃	ethyl acetate	3.40	s	CH ₃	1,2-dimethoxyethane	6.76	s	ArH	BHA
1.26	m	CH ₂	<i>n</i> -hexane	3.40	s	CH ₂	dimethyl malonate	6.83	m	CH(2,5)	pyrrole
1.26	br s	CH ₂	pump oil	3.48	q, 7	CH ₂	diethyl ether	6.98	s	ArH	BHT
1.27	m	CH ₂	<i>n</i> -pentane	3.49	s ⁹	CH ₃	methanol	7.10	s	CH(4,5)	imidazole
1.28	s	CH ₃	<i>tert</i> -butyl alcohol	3.55	s	CH ₂	1,2-dimethoxyethane	7.17	m	CH(2,4,6)	toluene
1.32	s ⁶	OH	ethanol	3.57	m	CH ₂	diglyme	7.25	m	CH(3,5)	toluene
1.32	sept, 7.3	CH ₂	propane	3.65	m	CH ₂	diglyme	7.26	s	CH	CDCl ₃ residual
1.43	s	ArC(CH ₃) ₃	BHT	3.67	s	CH ₂	18-crown-6	7.26	s	CH	chloroform
1.43	s	CH ₂	cyclohexane	3.71	s	CH ₂	1,4-dioxane	7.29	m	CH(3,5)	pyridine
1.44	s	ArC(CH ₃) ₃	BHA	3.72	q, 7 ⁹	CH ₂	ethanol	7.36	s	CH	benzene
1.56	s	OH	water	3.73	s	CH ₂	1,2-dichloroethane	7.45	dd	CH(2,5)	furan
1.68	m	CH ₂ (3,4)	pyrrolidine	3.75	s	CH ₃	dimethyl malonate	7.51–7.57	m	CH(3,5)	benzaldehyde
1.71–1.73	m	CH ₂ (4)	cyclohexanone	3.76	s	CH ₂	ethylene glycol	7.61–7.65	m	CH(4)	benzaldehyde
1.73	dt, 6.4, 1.5	CH ₃	propylene	3.76	m	CH ₂ (2,5)	tetrahydrofuran	7.67	s	CH(2)	imidazole
1.84–1.86	m	CH ₂ (3,5)	cyclohexanone	3.77	s	ArOCH ₃	BHA	7.68	m	CH(4)	pyridine
1.85	m	CH ₂ (3,4)	tetrahydrofuran	3.79	s	CH ₃	dimethyl carbonate	7.88–7.91	m	CH(2,6)	benzaldehyde
2.05	s	CH ₃ CO	ethyl acetate	4.04	sept, 6	CH	2-propanol	8.02	s	CH	dimethylformamide
2.09	s	CH ₃	allyl acetate	4.12	q, 7	CH ₂ CH ₃	ethyl acetate	8.40	br t	NH	pyrrole
2.09	s	CH ₃ CO	dimethylacetamide	4.33	s	CH ₃	nitromethane	8.62	m	CH(2,6)	pyridine
2.10	s	CH ₃	acetic acid	4.57	ddd	CH ₂	allyl acetate	10.03	s	HCO	benzaldehyde
2.10	s	CH ₃	acetonitrile	4.62	s	H ₂	hydrogen				

Table S8. CDCl₃ (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.63	CH ₄	methane	29.84	CH ₂	pump oil	64.50	CH	2-propanol	129.16	CH(3,5)	benzaldehyde
1.19	CH ₃	silicone grease	30.32	(CH ₃) ₃ C	BHA	65.28	CH ₂	allyl acetate	129.91	CH(2,6)	benzaldehyde
1.89	CH ₃	acetonitrile	30.33	(CH ₃) ₃ C	BHT	65.91	CH ₂	diethyl ether	131.58	CHCH ₂	diallyl carbonate
1.97	CH ₃	hexamethyldisiloxane	30.92	CH ₃	acetone	67.14	CH ₂	1,4-dioxane	132.21	C	hexamethylbenzene
6.89	CH ₃	ethane	31.25	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	67.97	CH ₂ (2,5)	tetrahydrofuran	132.33	CHCH ₂	allyl acetate
7.86	CH ₂ CH ₃	ethyl methyl ketone	31.45	CH ₃	dimethyl malonate	68.55	CH ₂	diallyl carbonate	133.91	CH	propylene
11.61	CH ₃	triethylamine	31.64	CH ₂ (3,4)	<i>n</i> -hexane	69.15	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	134.64	CH(4)	benzaldehyde
14.08	CH ₃	<i>n</i> -pentane	34.16	CH ₂ (3)	<i>n</i> -pentane	70.51	CH ₂	diglyme	135.38	CH(2)	imidazole
14.14	CH ₃	<i>n</i> -hexane	34.25	(CH ₃) ₃ C	BHT	70.55	CH ₂	18-crown-6	135.87	C(2,6)	BHT
14.19	CH ₃	ethyl acetate	34.72	(CH ₃) ₃ C	BHA	71.84	CH ₂	1,2-dimethoxyethane	135.96	CH(4)	pyridine
15.20	CH ₃	diethyl ether	35.28	NCH ₃	dimethylacetamide	71.90	CH ₂	diglyme	136.58	C(1)	benzaldehyde
16.37	CH ₂	propane	36.50	CH ₃	dimethyl malonate	77.16 (t)	CDCl ₃	CDCl ₃ signal	137.36	C(4)	BHA
16.63	CH ₃	propane	36.87 (d)	CH ₃	HMPA ¹	77.36	CH	chloroform	137.89	C(1)	toluene
16.98	CH ₃	hexamethylbenzene	36.89	CH ₂ CH ₃	ethyl methyl ketone	96.34	CCl ₄	carbon tetrachloride	142.71	CH(2,5)	furan
18.41	CH ₃	ethanol	38.13	NCH ₃	dimethylacetamide	107.98	CH(3,4)	pyrrole	147.85	C(2,6)	BHA
19.50	CH ₃	propylene	40.76	CH ₃	dimethyl sulfoxide	109.57	CH(3,4)	furan	149.90	CH(2,6)	pyridine
20.81	CH ₃	acetic acid	41.11	CH ₂	dimethyl malonate	110.69	CH(3,5)	BHA	151.55	C(1)	BHT
21.02	CH ₃	allyl acetate	41.97	CH ₂ (2,6)	cyclohexanone	115.74	CH ₂	propylene	152.57	C(1)	BHA
21.04	CH ₃ CO	ethyl acetate	43.50	CH ₂	1,2-dichloroethane	116.43	CN	acetonitrile	154.88	CO	diallyl carbonate
21.20	CH ₃ Ar	BHT	46.25	CH ₂	triethylamine	117.77	CH(2,5)	pyrrole	156.45	CO	dimethyl carbonate
21.46	CH ₃	toluene	46.93	CH ₂ (2,5)	pyrrolidine	118.34	CHCH ₂	allyl acetate	162.62	CH	dimethylformamide
21.53	CH ₃	dimethylacetamide	50.41	CH ₃	methanol	118.96	CHCH ₂	diallyl carbonate	167.18	CO ₂	dimethyl malonate
22.38	CH ₂ (2,4)	<i>n</i> -pentane	52.57	CH ₃	dimethyl malonate	122.00	CH(4,5)	imidazole	170.81	CO	allyl acetate
22.70	CH ₂ (2,5)	<i>n</i> -hexane	53.52	CH ₂	dichloromethane	123.13	CH ₂	ethylene	171.07	CO	dimethylacetamide
24.97	CH ₂ (4)	cyclohexanone	54.89	CH ₃	dimethyl carbonate	123.75	CH(3,5)	pyridine	171.36	CO	ethyl acetate
25.14	CH ₃	2-propanol	55.70	CH ₃ O	BHA	124.99	CO ₂	carbon dioxide	175.99	CO	acetic acid
25.56	CH ₃ (3,4)	pyrrolidine	58.28	CH ₂	ethanol	125.33	CH(4)	toluene	192.67	HCO	benzaldehyde
25.62	CH ₂ (3,4)	tetrahydrofuran	59.01	CH ₃	diglyme	125.55	CH(3,5)	BHT	192.83	CS ₂	carbon disulfide
26.94	CH ₂	cyclohexane	59.08	CH ₃	1,2-dimethoxyethane	128.26	CH(3,5)	toluene	207.07	CO	acetone
27.00	CH ₂ (3,5)	cyclohexanone	60.49	CH ₂	ethyl acetate	128.27	C(4)	BHT	209.56	CO	ethyl methyl ketone
29.49	CH ₃ CO	ethyl methyl ketone	62.50	CH ₃	nitromethane	128.37	CH	benzene	212.57	CO	cyclohexanone
29.71	CH ₂	H grease ⁸	63.79	CH ₂	ethylene glycol	129.07	CH(2,6)	toluene			

Table S9. Toluene- d_8 (^1H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.10	s	CH ₃	hexamethyldisiloxane	1.64	s	CH ₃	dimethyl sulfoxide	4.45	s	OH ^δ	BHA
0.17	s	CH ₄	methane	1.69	s	CH ₃ CO	ethyl acetate	4.50	s	H ₂	hydrogen
0.26	s	CH ₃	silicone grease	1.82	q, 7	CH ₂ CH ₃	ethyl methyl ketone	4.72	s	OH ^δ	BHT
0.43	s	OH	water	1.95	t	CH ₂ (2,6)	cyclohexanone	4.92	ddt	CHCH ₂ (2)	diallyl carbonate
0.58	s	OH	tert-butyl alcohol	1.96	s	CH ₃	dimethylformamide	4.92	dm, 10	CH ₂ (1)	propylene
0.69	s	CH ₃	acetonitrile	2.08	p	CH ₃	Toluene- d_8 residual	4.94	ddt	CHCH ₂ (2)	allyl acetate
0.81	s	CH ₃	ethane	2.10	s	CH ₃	hexamethylbenzene	4.98	dm, 17	CH ₂ (2)	propylene
0.83	s ^δ	OH	ethanol	2.11	s	NCH ₃	dimethylacetamide	5.05	ddt	CHCH ₂ (1)	allyl acetate
0.84	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.11	s	CH ₃	toluene	5.09	ddt	CHCH ₂ (1)	diallyl carbonate
0.87	t, 7	CH ₃	n-pentane	2.23	s	ArCH ₃	BHT	5.25	s	CH ₂	ethylene
0.88	t, 7	CH ₃	n-hexane	2.37	s	CH ₃	dimethylformamide	5.63	ddt	CHCH ₂	diallyl carbonate
0.88-0.96	m	CH ₃	pump oil	2.39	q, 7	CH ₂	triethylamine	5.67 ^f	(nfo ABX)	CHCH ₂	allyl acetate
0.89	t, 7,3	CH ₃	propane	2.42	d, 9,5	CH ₃	HMPA	5.70	m	CH	propylene
0.89-0.96	m	CH ₃	H grease ^g	2.54	m	CH ₂ (2,5)	pyrrolidine	6.07	dd	CH(3,4)	furan
0.94	t, 7	CH ₂ CH ₃	ethyl acetate	2.56	s	NCH ₃	dimethylacetamide	6.10	s	CH	chloroform
0.95	d, 6	CH ₃	2-propanol	2.91	s	CH ₂	1,2-dichloroethane	6.27	m	CH(3,4)	pyrrole
0.95	t, 7	CH ₃	triethylamine	2.92	s	CH ₂	dimethyl malonate	6.43	m	CH(2,5)	pyrrole
0.97	t, 7	CH ₃	ethanol	3.01	s	CH ₃	nitromethane	6.67	m	CH(3,5)	pyridine
1.03	s	CH ₃	tert-butyl alcohol	3.03	s ^δ	CH ₃	methanol	6.83	s	ArH	BHA
1.10	t, 7	CH ₃	diethyl ether	3.12	s	OCH ₃	diglyme	6.86	s	CH(4,5)	imidazole
1.16-1.20	m	CH ₂ (4)	cyclohexanone	3.12	s	CH ₃	1,2-dimethoxyethane	6.95-6.99	m	CH(3,5)	benzaldehyde
1.22	m	CH ₂	n-hexane	3.24	s	CH ₃	dimethyl malonate	6.96-7.01	m	CH(2,4,6)	toluene
1.25	m	CH ₂	n-pentane	3.25	q, 7	CH ₂	diethyl ether	6.97	p	CH(4)	Toluene- d_8 residual
1.30	br s	CH ₂	pump oil	3.31	m	CH ₂	diglyme	6.99	s	ArH	BHT
1.32	sept, 7,3	CH ₂	propane	3.31	s	CH ₂	1,2-dimethoxyethane	6.99	m	CH(4)	pyridine
1.33	br s	CH ₂	H grease ^g	3.31	s	CH ₃	dimethyl carbonate	7.01	s	CH(2,6)	Toluene- d_8 residual
1.33-1.39	m	CH ₂ (3,5)	cyclohexanone	3.33	s	CH ₂	1,4-dioxane	7.03-7.07	m	CH(4)	benzaldehyde
1.34	s	ArC(CH ₃) ₃	BHA	3.36	s	CH ₂	18-crown-6	7.09	m	CH(3,5)	Toluene- d_8 residual
1.36	s	ArC(CH ₃) ₃	BHT	3.36	q, 7 ^e	CH ₂	ethanol	7.09	m	CH(3,5)	toluene
1.36	m	CH ₂ (3,4)	pyrrolidine	3.36	s	CH ₂	ethylene glycol	7.10	dd	CH(2,5)	furan
1.40	s	CH ₂	cyclohexane	3.43	m	CH ₂	diglyme	7.12	s	CH	benzene
1.43	m	CH ₂ (3,4)	tetrahydrofuran	3.48	s	ArOCH ₃	BHA	7.30	s	CH(2)	imidazole
1.55	dt, 6,4, 1,5	CH ₃	propylene	3.54	m	CH ₂ (2,5)	tetrahydrofuran	7.45-7.47	m	CH(2,6)	benzaldehyde
1.57	s	CH ₃	acetic acid	3.65	sept, 6	CH	2-propanol	7.57	s	CH	dimethylformamide
1.57	s	CH ₃	acetone	3.87	q, 7	CH ₂ CH ₃	ethyl acetate	7.71	br t	NH	pyrrole
1.59	s	CH ₃ CO	dimethylacetamide	4.32	s	CH ₂	dichloromethane	8.47	m	CH(2,6)	pyridine
1.59	s	CH ₃ CO	ethyl methyl ketone	4.34	ddd	CH ₂	allyl acetate	9.57	s	HCO	benzaldehyde
1.63	s	CH ₃	allyl acetate	4.34	ddd	CH ₂	diallyl carbonate				

Table S10. Toluene- d_8 ($^{13}\text{C}\{^1\text{H}\}$ NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.34	CH ₄	methane	30.30	(CH ₃) ₃ C	BHA	64.87	CH ₂	allyl acetate	129.33	CH(2,6)	toluene
0.03	CH ₃	acetonitrile	30.31	CH ₂	H grease ^g	65.94	CH ₂	diethyl ether	129.61	CH(2,6)	benzaldehyde
1.37	CH ₃	silicone grease	30.33	CH ₂	pump oil	67.17	CH ₂	1,4-dioxane	131.72	C	hexamethylbenzene
1.99	CH ₃	hexamethyldisiloxane	30.49	(CH ₃) ₃ C	tert-butyl alcohol	67.75	CH ₂ (2,5)	tetrahydrofuran	132.30	CHCH ₂	diallyl carbonate
6.94	CH ₃	ethane	30.64	CH ₃	dimethylformamide	68.12	(CH ₃) ₃ C	tert-butyl alcohol	132.98	CHCH ₂	allyl acetate
7.89	CH ₂ CH ₃	ethyl methyl ketone	31.39	(CH ₃) ₃ C	BHT	68.20	CH ₂	diallyl carbonate	133.61	CH	propylene
12.39	CH ₃	triethylamine	32.06	CH ₂ (3,4)	n-hexane	70.86	CH ₂	18-crown-6	133.88	CH(4)	benzaldehyde
14.23	CH ₃	ethyl acetate	34.39	(CH ₃) ₃ C	BHT	70.92	CH ₂	diglyme	135.17	CH(4)	pyridine
14.27	CH ₃	n-pentane	34.54	CH ₂ (3)	n-pentane	72.25	CH ₂	1,2-dimethoxyethane	135.57	CH(2)	imidazole
14.34	CH ₃	n-hexane	34.58	NCH ₃	dimethylacetamide	72.39	CH ₂	diglyme	136.12	C(2,6)	BHT
15.47	CH ₃	diethyl ether	34.69	(CH ₃) ₃ C	BHA	77.89	CH	chloroform	137.12	C(1)	benzaldehyde
16.63	CH ₂	propane	35.22	CH ₃	dimethylformamide	96.57	CCl ₄	carbon tetrachloride	137.34	C(4)	BHA
16.65	CH ₃	propane	36.32	CH ₂ CH ₃	ethyl methyl ketone	108.15	CH(3,4)	pyrrole	137.48	C	toluene- d_8 signal
16.84	CH ₃	hexamethylbenzene	36.8 (d)	CH ₃	HMPA ^h	109.63	CH(3,4)	furan	137.84	C(1)	toluene
18.78	CH ₃	ethanol	36.98	NCH ₃	dimethylacetamide	110.99	CH(3,5)	BHA	142.65	CH(2,5)	furan
19.32	CH ₃	propylene	40.41	CH ₃	dimethyl sulfoxide	115.76	CN	acetonitrile	148.06	C(2,6)	BHA
20.21	CH ₃	allyl acetate	40.88	CH ₂	dimethyl malonate	115.89	CH ₂	propylene	150.25	CH(2,6)	pyridine
20.27	CH ₃	acetic acid	41.78	CH ₂ (2,6)	cyclohexanone	117.49	CHCH ₂	allyl acetate	152.06	C(1)	BHT
20.43 (sept)	CD ₃	toluene- d_8 signal	43.40	CH ₂	1,2-dichloroethane	117.61	CH(2,5)	pyrrole	153.50	C(1)	BHA
20.46	CH ₂ CO	ethyl acetate	46.82	CH ₂		118.04	CHCH ₂	diallyl carbonate	155.15	CO	diallyl carbonate
21.05	CH ₃	dimethylacetamide	47.12	CH ₂ (2,5)	pyrrolidine	122.13	CH(4,5)	imidazole	156.61	CO	dimethyl carbonate
21.37	CH ₃	toluene	49.90	CH ₃	methanol	122.92	CH ₂	ethylene	161.93	CH	dimethylformamide
21.42	CH ₃ Ar	BHT	51.76	CH ₃	dimethyl malonate	123.46	CH(3,5)	pyridine	166.49	CO ₂	dimethyl malonate
22.79	CH ₂ (2,4)	n-pentane	53.47	CH ₂	dichloromethane	124.86	CO ₂	carbon dioxide	169.44	CO	allyl acetate
23.12	CH ₂ (2,5)	n-hexane	54.13	CH ₃	dimethyl carbonate	125.13 (t)	CD(4)	toluene- d_8 signal	169.65	CO	dimethylacetamide
25.15	CH ₂ (4)	cyclohexanone	55.04	CH ₂ O	BHA	125.66	CH(4)	toluene	170.02	CO	ethyl acetate
25.24	CH ₃	2-propanol	57.81	CH ₂	ethanol	125.79	CH(3,5)	BHT	175.30	CO	acetic acid
25.75	CH ₂ (3,4)	pyrrolidine	58.62	CH ₃	diglyme	127.96 (t)	CD(3,5)	toluene- d_8 signal	191.09	HCO	benzaldehyde
25.79	CH ₂ (3,4)	tetrahydrofuran	58.63	CH ₃	1,2-dimethoxyethane	128.44	C(4)	BHT	192.71	CS ₂	carbon disulfide
27.05	CH ₂ (3,5)	cyclohexanone	60.08	CH ₂	ethyl acetate	128.51	CH(3,5)	toluene	204.00	CO	acetone
27.31	CH ₂	cyclohexane	61.14	CH ₃	nitromethane	128.57	CH	benzene	206.31	CO	ethyl methyl ketone
28.74	CH ₃ CO	ethyl methyl ketone	64.12	CH	2-propanol	128.68	CH(3,5)	benzaldehyde	208.60	CO	cyclohexanone
30.03	CH ₃	acetone	64.29	CH ₂	ethylene glycol	128.87 (t)	CD(2,6)	toluene- d_8 signal			

Table S11. C₆D₆ (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.12	s	CH ₃	hexamethyldisiloxane	1.63	s	CH ₃	allyl acetate	4.38	ddd	CH ₂	diallyl carbonate
0.16	s	CH ₄	methane	1.65	s	CH ₃ CO	ethyl acetate	4.47	s	H ₂	hydrogen
0.29	s	CH ₃	silicone grease	1.68	s	CH ₃	dimethyl sulfoxide	4.53	s	OH ^δ	BHA
0.40	s	OH	water	1.81	q, 7	CH ₂ CH ₃	ethyl methyl ketone	4.79	s	OH ^δ	BHT
0.50	s ⁶	OH	ethanol	1.86	s	CH ₃	dimethylformamide	4.92	ddt	CHCH ₂ (2)	diallyl carbonate
0.58	s	CH ₃	acetonitrile	1.98	t	CH ₂ (2,6)	cyclohexanone	4.94	ddt	CHCH ₂ (2)	allyl acetate
0.63	s	OH	tert-butyl alcohol	2.05	s	NCH ₃	dimethylacetamide	4.95	dm, 10	CH ₂ (1)	propylene
0.80	s	CH ₃	ethane	2.11	s	CH ₃	toluene	5.01	dm, 17	CH ₂ (2)	propylene
0.85	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.13	s	CH ₃	hexamethylbenzene	5.06	ddt	CHCH ₂ (1)	allyl acetate
0.86	t, 7, 3	CH ₃	propane	2.24	s	ArCH ₃	BHT	5.09	ddt	CHCH ₂ (1)	diallyl carbonate
0.87	t, 7	CH ₃	n-pentane	2.36	s	CH ₃	dimethylformamide	5.25	s	CH ₂	ethylene
0.89	t, 7	CH ₃	n-hexane	2.40	d, 9, 5	CH ₃	HMPA	5.65	ddt	CHCH ₂	diallyl carbonate
0.90–0.98	m	CH ₃	H grease ⁸	2.40	q, 7	CH ₂	triethylamine	5.68 ⁷	t(nfo ABX)	CHCH ₂	allyl acetate
0.91–0.97	m	CH ₃	pump oil	2.54	m	CH ₂ (2,5)	pyrrolidine	5.72	m	CH	propylene
0.92	t, 7	CH ₂ CH ₃	ethyl acetate	2.57	s	NCH ₃	dimethylacetamide	6.08	dd	CH(3,4)	uran
0.95	d, 6	CH ₃	2-propanol	2.90	s	CH ₂	1,2-dichloroethane	6.15	s	CH	chloroform
0.96	t, 7	CH ₃	ethanol	2.94	s	CH ₃	nitromethane	6.37	m	CH(3,4)	pyrrole
0.96	t, 7	CH ₃	triethylamine	2.97	s	CH ₂	dimethyl malonate	6.48	m	CH(2,5)	pyrrole
1.05	s	CH ₃	tert-butyl alcohol	3.07	s ⁹	CH ₃	methanol	6.66	m	CH(3,5)	pyridine
1.08–1.16	m	CH ₂ (4)	cyclohexanone	3.11	s	OCH ₃	diglyme	6.90	s	CH(4,5)	imidazole
1.11	t, 7	CH ₃	diethyl ether	3.12	s	CH ₃	1,2-dimethoxyethane	6.93	s	ArH	BHA
1.23	m	CH ₂	n-pentane	3.23	s	CH ₃	dimethyl malonate	6.93–6.99	m	CH(3,5)	benzaldehyde
1.24	m	CH ₂	n-hexane	3.26	q, 7	CH ₂	diethyl ether	6.98	m	CH(4)	pyridine
1.26	sept, 7, 3	CH ₂	propane	3.30	s	CH ₃	dimethyl carbonate	7.01–7.07	m	CH(4)	benzaldehyde
1.28–1.37	m	CH ₂ (3,5)	cyclohexanone	3.33	s	CH ₂	1,2-dimethoxyethane	7.02	m	CH(2,4,6)	toluene
1.32	br s	CH ₂	H grease ⁸	3.34	m	CH ₂	diglyme	7.05	s	ArH	BHT
1.33	m	CH ₂ (3,4)	pyrrolidine	3.34	q, 7 ⁶	CH ₂	ethanol	7.13	dd	CH(2,5)	furan
1.37	br s	CH ₂	pump oil	3.35	s	CH ₂	1,4-dioxane	7.13	m	CH(3,5)	toluene
1.38	s	ArC(CH ₃) ₃	BHT	3.39	s	CH ₂	18-crown-6	7.15	s	CH	benzene
1.40	s	CH ₂	cyclohexane	3.41	s	CH ₂	ethylene glycol	7.16	s	CH	C ₆ D ₆ residual
1.40	m	CH ₂ (3,4)	tetrahydrofuran	3.46	m	CH ₂	diglyme	7.33	s	CH(2)	imidazole
1.41	s	ArC(CH ₃) ₃	BHA	3.48	m	ArOCH ₃	BHA	7.49–7.53	m	CH(2,6)	benzaldehyde
1.52	s	CH ₃	acetic acid	3.57	m	CH ₂ (2,5)	tetrahydrofuran	7.63	s	CH	dimethylformamide
1.55	s	CH ₃	acetone	3.67	sept, 6	CH	2-propanol	7.80	br t	NH	pyrrole
1.55	dt, 6, 4, 1, 5	CH ₃	propylene	3.89	q, 7	CH ₂ CH ₃	ethyl acetate	8.53	m	CH(2,6)	pyridine
1.58	s	CH ₃ CO	ethyl methyl ketone	4.27	s	CH ₂	dichloromethane	9.64	s	HCO	benzaldehyde
1.60	s	CH ₃ CO	dimethylacetamide	4.38	ddd	CH ₂	allyl acetate				

Table S12. C₆D₆ (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.29	CH ₄	methane	30.22	CH ₂	H grease ⁸	64.34	CH ₂	ethylene glycol	129.33	CH(2,6)	toluene
0.20	CH ₃	acetonitrile	30.24	CH ₂	pump oil	64.92	CH ₂	allyl acetate	129.65	CH(2,6)	benzaldehyde
1.38	CH ₃	silicone grease	30.35	(CH ₃) ₃ C	BHA	65.94	CH ₂	diethyl ether	131.79	C	hexamethylbenzene
2.05	CH ₃	hexamethyldisiloxane	30.47	(CH ₃) ₃ C	tert-butyl alcohol	67.16	CH ₂	1,4-dioxane	132.18	CHCH ₂	diallyl carbonate
6.96	CH ₃	ethane	30.72	CH ₃	dimethylformamide	67.80	CH ₂ (2,5)	tetrahydrofuran	132.90	CHCH ₂	allyl acetate
7.91	CH ₂ CH ₃	ethyl methyl ketone	31.34	(CH ₃) ₃ C	BHT	68.19	(CH ₃) ₃ C	tert-butyl alcohol	133.69	CH	propylene
12.35	CH ₃	triethylamine	31.96	CH ₂ (3,4)	n-hexane	68.28	CH ₂	diallyl carbonate	133.95	CH(4)	benzaldehyde
14.19	CH ₃	ethyl acetate	34.35	(CH ₃) ₃ C	BHT	70.59	CH ₂	18-crown-6	135.28	CH(4)	pyridine
14.25	CH ₃	n-pentane	34.45	CH ₂ (3)	n-pentane	70.87	CH ₂	diglyme	135.76	CH(2)	imidazole
14.32	CH ₃	n-hexane	34.67	NCH ₃	dimethylacetamide	72.21	CH ₂	1,2-dimethoxyethane	136.08	C(2,6)	BHT
15.46	CH ₃	diethyl ether	34.72	(CH ₃) ₃ C	BHA	72.35	CH ₂	diglyme	137.05	C(1)	benzaldehyde
16.60	CH ₂	propane	35.25	CH ₃	dimethylformamide	77.79	CH	chloroform	137.50	C(4)	BHA
16.66	CH ₃	propane	36.36	CH ₂ CH ₃	ethyl methyl ketone	96.44	CCl ₄	carbon tetrachloride	137.91	C(1)	toluene
16.95	CH ₃	hexamethylbenzene	36.88 (d)	CH ₃	HMPA ¹¹	108.21	CH(3,4)	pyrrole	142.73	CH(2,5)	furan
18.72	CH ₃	ethanol	37.03	NCH ₃	dimethylacetamide	109.67	CH(3,4)	furan	148.13	C(2,6)	BHA
19.38	CH ₃	propylene	40.03	CH ₃	dimethyl sulfoxide	111.15	CH(3,5)	BHA	150.27	CH(2,6)	pyridine
20.37	CH ₃	acetic acid	41.04	CH ₂	dimethyl malonate	115.92	CH ₂	propylene	152.05	C(1)	BHT
20.37	CH ₃	allyl acetate	41.83	CH ₂ (2,6)	cyclohexanone	116.02	CN	acetonitrile	153.62	C(1)	BHA
20.56	CH ₃ CO	ethyl acetate	43.59	CH ₂	1,2-dichloroethane	117.64	CHCH ₂	allyl acetate	155.24	CO	diallyl carbonate
21.10	CH ₃	toluene	46.77	CH ₂	triethylamine	117.78	CH(2,5)	pyrrole	156.71	CO	dimethyl carbonate
21.16	CH ₃	dimethylacetamide	46.86	CH ₂ (2,5)	pyrrolidine	118.22	CHCH ₂	diallyl carbonate	162.13	CH	dimethylformamide
21.40	CH ₂ Ar	BHT	49.97	CH ₃	methanol	122.16	CH(4,5)	imidazole	166.66	CO ₂	dimethyl malonate
22.72	CH ₂ (2,4)	n-pentane	51.86	CH ₃	dimethyl malonate	122.96	CH ₂	ethylene	169.67	CO	allyl acetate
23.04	CH ₂ (2,5)	n-hexane	53.46	CH ₂	dichloromethane	123.58	CH(3,5)	pyridine	169.95	CO	dimethylacetamide
25.03	CH ₂ (4)	cyclohexanone	54.30	CH ₃	dimethyl carbonate	124.76	CO ₂	carbon dioxide	170.44	CO	ethyl acetate
25.18	CH ₃	2-propanol	55.27	CH ₃ O	BHA	125.68	CH(4)	toluene	175.82	CO	acetic acid
25.65	CH ₂ (3,4)	pyrrolidine	57.86	CH ₂	ethanol	125.83	CH(3,5)	BHT	191.43	HCO	benzaldehyde
25.72	CH ₂ (3,4)	tetrahydrofuran	58.66	CH ₃	diglyme	128.06 (t)	CD	C ₆ D ₆ signal	192.69	CS ₂	carbon disulfide
27.00	CH ₂ (3,5)	cyclohexanone	58.68	CH ₃	1,2-dimethoxyethane	128.52	C(4)	BHT	204.43	CO	acetone
27.23	CH ₂	cyclohexane	60.21	CH ₂	ethyl acetate	128.56	CH(3,5)	toluene	206.55	CO	ethyl methyl ketone
28.56	CH ₃ CO	ethyl methyl ketone	61.16	CH ₃	nitromethane	128.62	CH	benzene	209.10	CO	cyclohexanone
30.14	CH ₃	acetone	64.23	CH	2-propanol	128.95	CH(3,5)	benzaldehyde			

Table S13. C₆D₅Cl (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.10	s	CH ₃	hexamethyldisiloxane	1.78	s	CH ₃ CO	ethyl methyl ketone	4.62	s	OH ^δ	BHA
0.14	s	CH ₃	silicone grease	1.80	s	CH ₃	allyl acetate	4.77	s	CH ₂	dichloromethane
0.15	s	CH ₄	methane	2.03	s	CH ₃	dimethyl sulfoxide	4.91	dm, 10	CH ₂ (1)	propylene
0.79	s	CH ₃	ethane	2.06	q, 7	CH ₂ CH ₃	ethyl methyl ketone	4.98	dm, 17	CH ₂ (2)	propylene
0.84	t, 7	CH ₃	<i>n</i> -pentane	2.08	t	CH ₂ (2,6)	cyclohexanone	5.03	ddt	CHCH ₂ (2)	diallyl carbonate
0.84	t, 7,3	CH ₃	propane	2.10	s	CH ₃	hexamethylbenzene	5.04	ddt	CHCH ₂ (2)	allyl acetate
0.85	t, 7	CH ₃	<i>n</i> -hexane	2.16	s	CH ₃	toluene	5.15	ddt	CHCH ₂ (1)	allyl acetate
0.86-0.92	m	CH ₃	H grease ^δ	2.20	s	ArCH ₃	BHT	5.17	ddt	CHCH ₂ (1)	diallyl carbonate
0.88-0.91	m	CH ₃	pump oil	2.30	s	CH ₃	dimethylformamide	5.29	s	CH ₂	ethylene
0.89	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.39	q, 7	CH ₂	triethylamine	5.50	s	OH ^δ	BHT
0.93	t, 7	CH ₃	triethylamine	2.42	s	NCH ₃	dimethylacetamide	5.72	m	CH	propylene
1.03	s	OH	water	2.47	d, 9,5	CH ₃	HMPA	5.75	ddt	CHCH ₂	diallyl carbonate
1.04	t, 7	CH ₂ CH ₃	ethyl acetate	2.51	s	CH ₃	dimethylformamide	5.77	ddt	CHCH ₂	allyl acetate
1.04	d, 6	CH ₃	2-propanol	2.64	m	CH ₂ (2,5)	pyrrolidine	6.19	dd	CH(3,4)	furan
1.06	t, 7	CH ₃	ethanol	2.65	s	NCH ₃	dimethylacetamide	6.27	m	CH(3,4)	pyrrole
1.10	t, 7	CH ₃	diethyl ether	3.15	s	CH ₂	dimethyl malonate	6.62	m	CH(2,5)	pyrrole
1.12	s	CH ₃	<i>tert</i> -butyl alcohol	3.16	s	OCH ₃	diglyme	6.74	s	CH	chloroform
1.19	m	CH ₂	<i>n</i> -hexane	3.17	s	CH ₃	1,2-dimethoxyethane	6.83	s	ArH	BHA
1.21	s	CH ₃	acetonitrile	3.25	s ^δ	CH ₃	methanol	6.90	m	CH(3,5)	pyridine
1.23	m	CH ₂	<i>n</i> -pentane	3.26	s	CH ₂	1,2-dichloroethane	6.96	br. s	CH(4)	C ₆ D ₅ Cl residual
1.26	sept, 7,3	CH ₂	propane	3.31	q, 7	CH ₂	diethyl ether	6.97	s	ArH	BHT
1.30	s	OH	<i>tert</i> -butyl alcohol	3.37	m	CH ₂	diglyme	6.99	br. s	CH(3,5)	C ₆ D ₅ Cl residual
1.30	br s	CH ₂	H grease ^δ	3.37	s	CH ₂	1,2-dimethoxyethane	7.01	s	CH(4,5)	imidazole
1.30	s ^δ	OH	methanol	3.41	s	CH ₂	18-crown-6	7.01-7.08	m	CH(2,4,6)	toluene
1.31	br s	CH ₂	pump oil	3.41	s	CH ₃	dimethyl malonate	7.10-7.17	m	CH(3,5)	toluene
1.33-1.37	m	CH ₂ (4)	cyclohexanone	3.45	s	CH ₂	1,4-dioxane	7.14	br. s	CH(2,6)	C ₆ D ₅ Cl residual
1.37	s	ArC(CH ₃) ₃	BHA	3.48	s	CH ₃	dimethyl carbonate	7.15-7.19	m	CH(3,5)	benzaldehyde
1.37	s	ArC(CH ₃) ₃	BHT	3.49	m	CH ₂	diglyme	7.20	s	CH	benzene
1.37	s	CH ₂	cyclohexane	3.51	q, 7 ^δ	CH ₂	ethanol	7.24	dd	CH(2,5)	furan
1.39	s ^δ	OH	ethanol	3.58	s	CH ₂	ethylene glycol	7.24-7.28	m	CH(4)	benzaldehyde
1.43	m	CH ₂ (3,4)	pyrrolidine	3.59	s	CH ₃	nitromethane	7.25	m	CH(4)	pyridine
1.48-1.53	m	CH ₂ (3,5)	cyclohexanone	3.59	m	CH ₂ (2,5)	tetrahydrofuran	7.53	s	CH(2)	imidazole
1.55	m	CH ₂ (3,4)	tetrahydrofuran	3.61	s	ArOCH ₃	BHA	7.59-7.61	m	CH(2,6)	benzaldehyde
1.58	dt, 6,4, 1,5	CH ₃	propylene	3.82	sept, 6	CH	2-propanol	7.73	s	CH	dimethylformamide
1.74	s	CH ₃ CO	dimethylacetamide	3.96	q, 7	CH ₂ CH ₃	ethyl acetate	8.51	m	CH(2,6)	pyridine
1.76	s	CH ₃	acetic acid	4.44	ddd	CH ₂	allyl acetate	8.61	br t	NH	pyrrole
1.77	s	CH ₃	acetone	4.46	ddd	CH ₂	diallyl carbonate	9.77	s	HCO	benzaldehyde
1.78	s	CH ₃ CO	ethyl acetate	4.49	s	H ₂	hydrogen				

Table S14. C₆D₅Cl (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.33	CH ₄	methane	30.12	CH ₃	acetone	65.79	CH ₂	diethyl ether	129.26 (t)	CD(2,6)	C ₆ D ₅ Cl signal
0.63	CH ₃	acetonitrile	30.19	(CH ₃) ₃ C	BHT	66.95	CH ₂	1,4-dioxane	129.49	CH(2,6)	benzaldehyde
1.09	CH ₃	silicone grease	30.21	(CH ₃) ₃ C	BHA	67.64	CH ₂ (2,5)	tetrahydrofuran	131.54	C	hexamethylbenzene
1.92	CH ₃	hexamethyldisiloxane	30.71	CH ₃	dimethylformamide	68.19	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	131.93	CHCH ₂	diallyl carbonate
6.91	CH ₃	ethane	31.13	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	68.19	CH ₂	diallyl carbonate	132.69	CHCH ₂	allyl acetate
7.79	CH ₂ CH ₃	ethyl methyl ketone	31.77	CH ₂ (3,4)	<i>n</i> -hexane	70.55	CH ₂	18-crown-6	133.57	CH	propylene
11.87	CH ₃	triethylamine	34.11	(CH ₃) ₃ C	BHT	70.56	CH ₂	diglyme	134.02	CH(4)	benzaldehyde
14.07	CH ₃	ethyl acetate	34.26	CH ₂ (3)	<i>n</i> -pentane	71.81	CH ₂	1,2-dimethoxyethane	134.19	CCl	C ₆ D ₅ Cl signal
14.10	CH ₃	<i>n</i> -pentane	34.56	(CH ₃) ₃ C	BHA	72.07	CH ₂	diglyme	135.32	CH(4)	pyridine
14.18	CH ₃	<i>n</i> -hexane	34.59	NCH ₃	dimethylacetamide	77.67	CH	chloroform	135.50	CH(2)	imidazole
15.35	CH ₃	diethyl ether	35.45	CH ₃	dimethylformamide	96.38	CCl ₄	carbon tetrachloride	135.92	C(2,6)	BHT
16.48	CH ₂	propane	36.39	CH ₂ CH ₃	ethyl methyl ketone	108.03	CH(3,4)	pyrrole	136.78	C(1)	benzaldehyde
16.56	CH ₃	propane	36.64 (d)	CH ₃	HMPA ¹⁷	109.64	CH(3,4)	furan	137.29	C(4)	BHA
16.68	CH ₃	hexamethylbenzene	37.13	NCH ₃	dimethylacetamide	110.84	CH(3,5)	BHA	137.65	C(1)	toluene
18.55	CH ₃	ethanol	40.27	CH ₃	dimethyl sulfoxide	115.86	CH ₂	propylene	142.49	CH(2,5)	furan
19.32	CH ₃	propylene	40.93	CH ₂	dimethyl malonate	115.93	CN	acetonitrile	147.87	C(2,6)	BHA
20.40	CH ₃	acetic acid	41.79	CH ₂ (2,6)	cyclohexanone	117.63	CHCH ₂	allyl acetate	149.93	CH(2,6)	pyridine
20.40	CH ₃	allyl acetate	43.60	CH ₂	1,2-dichloroethane	117.65	CH(2,5)	pyrrole	151.69	C(1)	BHT
20.50	CH ₃ CO	ethyl acetate	46.36	CH ₂	triethylamine	118.22	CHCH ₂	diallyl carbonate	153.19	C(1)	BHA
21.03	CH ₃	dimethylacetamide	46.75	CH ₂ (2,5)	pyrrolidine	121.96	CH(4,5)	imidazole	154.87	CO	diallyl carbonate
21.10	CH ₂ Ar	BHT	49.66	CH ₃	methanol	122.95	CH ₂	ethylene	156.36	CO	dimethyl carbonate
21.23	CH ₃	toluene	51.89	CH ₃	dimethyl malonate	123.49	CH(3,5)	pyridine	162.01	CH	dimethylformamide
22.54	CH ₂ (2,4)	<i>n</i> -pentane	53.54	CH ₂	dichloromethane	125.43	CH(4)	toluene	166.51	CO ₂	dimethyl malonate
22.86	CH ₂ (2,5)	<i>n</i> -hexane	54.23	CH ₃	dimethyl carbonate	125.58	CH(3,5)	BHT	169.59	CO	allyl acetate
25.07	CH ₂ (4)	cyclohexanone	55.08	CH ₃ O	BHA	125.96 (t)	CD(4)	C ₆ D ₅ Cl signal	169.79	CO	dimethylacetamide
25.14	CH ₃	2-propanol	57.63	CH ₂	ethanol	126.08	CO ₂	carbon dioxide	170.20	CO	ethyl acetate
25.59	CH ₂ (3,4)	pyrrolidine	58.31	CH ₃	1,2-dimethoxyethane	128.25 (t)	CD(3,5)	C ₆ D ₅ Cl signal	175.67	CO	acetic acid
25.68	CH ₂ (3,4)	tetrahydrofuran	58.42	CH ₃	diglyme	128.26	C(4)	BHT	191.24	HCO	benzaldehyde
26.99	CH ₂	cyclohexane	60.06	CH ₂	ethyl acetate	128.31	CH(3,5)	toluene	192.49	CS ₂	carbon disulfide
27.02	CH ₂ (3,5)	cyclohexanone	61.68	CH ₃	nitromethane	128.38	CH	benzene	204.83	CO	acetone
28.82	CH ₃ CO	ethyl methyl ketone	64.03	CH ₂	ethylene glycol	128.87	CH(3,5)	benzaldehyde	206.87	CO	ethyl methyl ketone
30.11	CH ₂	H grease ^δ	64.18	CH	2-propanol	129.12	CH(2,6)	toluene	209.30	CO	cyclohexanone
30.11	CH ₂	pump oil	64.86	CH ₂	allyl acetate						

Table S15. (CD₃)₂CO (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.07	s	CH ₃	hexamethyldisiloxane	2.17	s	CH ₃	hexamethylbenzene	4.54	s	H ₂	hydrogen
0.13	s	CH ₃	silicone grease	2.22	s	ArCH ₃	BHT	4.62	ddd	CH ₂	diallyl carbonate
0.17	s	CH ₄	methane	2.27	t	CH ₂ (2,6)	cyclohexanone	4.90	dm, 10	CH ₂ (1)	propylene
0.83	s	CH ₃	ethane	2.32	s	CH ₃	toluene	5.00	dm, 17	CH ₂ (2)	propylene
0.87	m	CH ₃	pump oil	2.45	q, 7	CH ₂ CH ₃	ethyl methyl ketone	5.18	ddt	CHCH ₂ (2)	allyl acetate
0.88	t, 7	CH ₃	<i>n</i> -hexane	2.45	q, 7	CH ₂	triethylamine	5.23	ddt	CHCH ₂ (2)	diallyl carbonate
0.88	t, 7	CH ₃	<i>n</i> -pentane	2.52	s	CH ₃	dimethyl sulfoxide	5.29	ddt	CHCH ₂ (1)	allyl acetate
0.88	t, 7.3	CH ₃	propane	2.59	d, 9.5	CH ₃	HMPA	5.35	ddt	CHCH ₂ (1)	diallyl carbonate
0.90	m	CH ₃	H grease ⁸	2.78	s	CH ₃	dimethylformamide	5.38	s	CH ₂	ethylene
0.96	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.83	s	NCH ₃	dimethylacetamide	5.63	s	CH ₂	dichloromethane
0.96	t, 7	CH ₃	triethylamine	2.84 ³	s	OH	water	5.65	s	OH ⁵	BHA
1.10	d, 6	CH ₃	2-propanol	2.94	s	CH ₃	dimethylformamide	5.81	m	CH	propylene
1.11	t, 7	CH ₃	diethyl ether	3.00	s	NCH ₃	dimethylacetamide	5.92	ddt	CHCH ₂	allyl acetate
1.12	t, 7	CH ₃	ethanol	3.12	s ⁹	OH	methanol	5.96	ddt	CHCH ₂	diallyl carbonate
1.18	s	CH ₃	<i>tert</i> -butyl alcohol	3.28	s	OCH ₃	diglyme	6.07	m	CH(3,4)	pyrrole
1.20	t, 7	CH ₂ CH ₃	ethyl acetate	3.28	s	CH ₃	1,2-dimethoxyethane	6.43	dd	CH(3,4)	furan
1.27	m	CH ₂	<i>n</i> -pentane	3.28	s	CH ₂	ethylene glycol	6.72	s	ArH	BHA
1.28	m	CH ₂	<i>n</i> -hexane	3.31	s ⁹	CH ₃	methanol	6.77	m	CH(2,5)	pyrrole
1.29	br s	CH ₂	H grease ⁸	3.39	s ⁶	OH	ethanol	6.96	s	ArH	BHT
1.29	br s	CH ₂	pump oil	3.41	q, 7	CH ₂	diethyl ether	7.04	s	CH(4,5)	imidazole
1.31	sept, 7.3	CH ₂	propane	3.42	s	CH ₂	dimethyl malonate	7.10–7.20	m	CH(2,4,6)	toluene
1.41	s	ArC(CH ₃) ₃	BHA	3.46	s	CH ₂	1,2-dimethoxyethane	7.10–7.20	m	CH(3,5)	toluene
1.41	s	ArC(CH ₃) ₃	BHT	3.47	m	CH ₂	diglyme	7.35	m	CH(3,5)	pyridine
1.43	s	CH ₂	cyclohexane	3.56	m	CH ₂	diglyme	7.36	s	CH	benzene
1.68	dt, 6.4, 1.5	CH ₃	propylene	3.57	q, 7 ⁶	CH ₂	ethanol	7.56	dd	CH(2,5)	furan
1.70–1.74	m	CH ₂ (4)	cyclohexanone	3.59	s	CH ₂	18-crown-6	7.59–7.63	m	CH(3,5)	benzaldehyde
1.79	m	CH ₂ (3,4)	tetrahydrofuran	3.59	s	CH ₂	1,4-dioxane	7.62	s	CH(2)	imidazole
1.79–1.83	m	CH ₂ (3,5)	cyclohexanone	3.63	m	CH ₂ (2,5)	tetrahydrofuran	7.69–7.73	m	CH(4)	benzaldehyde
1.96	s	CH ₃	acetic acid	3.68	s	CH ₃	dimethyl malonate	7.76	m	CH(4)	pyridine
1.97	s	CH ₂ CO	dimethylacetamide	3.72	s	ArOCH ₃	BHA	7.92–7.94	m	CH(2,6)	benzaldehyde
1.97	s	CH ₂ CO	ethyl acetate	3.72	s	CH ₃	dimethyl carbonate	7.96	s	CH	dimethylformamide
2.02	s	CH ₃	allyl acetate	3.87	s	CH ₂	1,2-dichloroethane	8.02	s	CH	chloroform
2.05	s	CH ₃	acetonitrile	3.90	sept, 6	CH	2-propanol	8.58	m	CH(2,6)	pyridine
2.05	p	CHD ₂	(CD ₃) ₂ CO residual	4.05	q, 7	CH ₂ CH ₃	ethyl acetate	10.02	br t	NH	pyrrole
2.07	s	CH ₂ CO	ethyl methyl ketone	4.43	s	CH ₃	nitromethane	10.05	s	HCO	benzaldehyde
2.09	s	CH ₃	acetone	4.53	ddd	CH ₂	allyl acetate				

Table S16. (CD₃)₂CO (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-5.33	CH ₄	methane	30.60	CH ₃	acetone	65.28	CH ₂	allyl acetate	130.23	CH(2,6)	benzaldehyde
1.12	CH ₃	acetonitrile	30.64	(CH ₃) ₃ C	BHA	66.12	CH ₂	diethyl ether	132.22	C	hexamethylbenzene
1.40	CH ₃	silicone grease	30.72	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	67.60	CH ₂	1,4-dioxane	133.16	CHCH ₂	diallyl carbonate
2.01	CH ₃	hexamethyldisiloxane	31.03	CH ₃	dimethylformamide	68.07	CH ₂ (2,5)	tetrahydrofuran	133.76	CHCH ₂	allyl acetate
6.88	CH ₃	ethane	31.61	(CH ₃) ₃ C	BHT	68.13	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	134.34	CH	propylene
8.03	CH ₂ CH ₃	ethyl methyl ketone	32.30	CH ₂ (3,4)	<i>n</i> -hexane	68.78	CH ₂	diallyl carbonate	135.14	CH(4)	benzaldehyde
12.49	CH ₃	triethylamine	34.83	CH ₂ (3)	<i>n</i> -pentane	71.03	CH ₂	diglyme	135.89	CH(2)	imidazole
14.29	CH ₃	<i>n</i> -pentane	34.89	NCH ₃	dimethylacetamide	71.25	CH ₂	18-crown-6	136.56	CH(4)	pyridine
14.34	CH ₃	<i>n</i> -hexane	35.00	(CH ₃) ₃ C	BHT	72.47	CH ₂	1,2-dimethoxyethane	137.66	C(1)	benzaldehyde
14.50	CH ₃	ethyl acetate	35.45	(CH ₃) ₃ C	BHA	72.63	CH ₂	diglyme	138.19	C(2,6)	BHT
15.78	CH ₃	diethyl ether	36.15	CH ₃	dimethylformamide	79.19	CH	chloroform	138.48	C(1)	toluene
16.68	CH ₃	propane	36.75	CH ₂ CH ₃	ethyl methyl ketone	96.65	CCl ₄	carbon tetrachloride	140.32	CH(4)	BHA
16.78	CH ₂	propane	37.04 (d)	CH ₃	HMPA ¹¹	108.04	CH(3,4)	pyrrole	143.49	CH(2,5)	furan
16.86	CH ₃	hexamethylbenzene	37.92	NCH ₃	dimethylacetamide	110.24	CH(3,4)	furan	148.48	C(2,6)	BHA
18.89	CH ₃	ethanol	41.23	CH ₃	dimethyl sulfoxide	111.00	CH(3,5)	BHA	150.67	CH(2,6)	pyridine
19.42	CH ₃	propylene	41.43	CH ₂	dimethyl malonate	116.03	CH ₂	propylene	152.51	C(1)	BHT
20.51	CH ₃	acetic acid	42.24	CH ₂ (2,6)	cyclohexanone	117.60	CN	acetonitrile	153.97	C(1)	BHA
20.68	CH ₃	allyl acetate	45.25	CH ₂	1,2-dichloroethane	117.81	CHCH ₂	allyl acetate	155.48	CO	diallyl carbonate
20.83	CH ₂ CO	ethyl acetate	47.07	CH ₂	triethylamine	117.98	CH(2,5)	pyrrole	157.04	CO	dimethyl carbonate
21.31	CH ₃ Ar	BHT	49.77	CH ₃	methanol	118.53	CHCH ₂	diallyl carbonate	162.79	CH	dimethylformamide
21.46	CH ₃	toluene	52.47	CH ₃	dimethyl malonate	122.31	CH(4,5)	imidazole	167.58	CO ₂	dimethyl malonate
21.51	CH ₃	dimethylacetamide	54.95	CH ₂	dichloromethane	123.47	CH ₂	ethylene	170.61	CO	allyl acetate
22.98	CH ₂ (2,4)	<i>n</i> -pentane	54.95	CH ₃	dimethyl carbonate	124.57	CH(3,5)	pyridine	170.61	CO	dimethylacetamide
23.28	CH ₂ (2,5)	<i>n</i> -hexane	55.51	CH ₃ O	BHA	125.81	CO ₂	carbon dioxide	170.96	CO	ethyl acetate
25.59	CH ₂ (4)	cyclohexanone	57.72	CH ₂	ethanol	126.03	CH(3,5)	BHT	172.31	CO	acetic acid
25.67	CH ₃	2-propanol	58.45	CH ₃	1,2-dimethoxyethane	126.12	CH(4)	toluene	192.95	HCO	benzaldehyde
26.15	CH ₂ (3,4)	tetrahydrofuran	58.77	CH ₃	diglyme	129.03	CH(3,5)	toluene	193.58	CS ₂	carbon disulfide
27.51	CH ₂	cyclohexane	60.56	CH ₂	ethyl acetate	129.05	C(4)	BHT	205.87	CO	acetone
27.68	CH ₂ (3,5)	cyclohexanone	63.21	CH ₃	nitromethane	129.15	CH	benzene	206.26	CO	(CD ₃) ₂ CO signal
29.30	CH ₂ CO	ethyl methyl ketone	63.85	CH	2-propanol	129.76	CH(2,6)	toluene	208.30	CO	ethyl methyl ketone
29.84 (sept)	CD ₃	(CD ₃) ₂ CO signal	64.26	CH ₂	ethylene glycol	129.90	CH(3,5)	benzaldehyde	210.36	CO	cyclohexanone
30.36	CH ₂	pump oil									

Table S17. (CD₃)₂SO (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
-0.06	s	CH ₃	silicone grease	2.18	s	ArCH ₃	BHT	4.61	ddd	CH ₂	diallyl carbonate
0.06	s	CH ₃	hexamethyldisiloxane	2.25	t	CH ₂ (2,6)	cyclohexanone	4.61	s	H ₂	hydrogen
0.20	s	CH ₄	methane	2.30	s	CH ₃	toluene	4.63	s ⁵	OH	ethanol
0.74	m	CH ₃	pump oil	2.43	q, 7	CH ₂ CH ₃	ethyl methyl ketone	4.94	dm, 10	CH ₂ (1)	propylene
0.82	s	CH ₃	ethane	2.43	q, 7	CH ₂	triethylamine	5.03	dm, 17	CH ₂ (2)	propylene
0.82-0.88	m	CH ₃	H grease ⁸	2.50	p	CHD ₂	(CD ₃) ₂ SO residual	5.20	ddt	CHCH ₂ (2)	allyl acetate
0.86	t, 7	CH ₃	<i>n</i> -hexane	2.53	d, 9,5	CH ₃	HMPA	5.25	ddt	CHCH ₂ (2)	diallyl carbonate
0.86	t, 7	CH ₃	<i>n</i> -pentane	2.54	s	CH ₃	dimethyl sulfoxide	5.29	ddt	CHCH ₂ (1)	allyl acetate
0.87	t, 7,3	CH ₃	propane	2.67	m	CH ₂ (2,5)	pyrrolidine	5.33	ddt	CHCH ₂ (1)	diallyl carbonate
0.91	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.73	s	CH ₃	dimethylformamide	5.41	s	CH ₂	ethylene
0.93	t, 7	CH ₃	triethylamine	2.78	s	NCH ₃	dimethylacetamide	5.76	s	CH ₂	dichloromethane
1.04	d, 6	CH ₃	2-propanol	2.89	s	CH ₃	dimethylformamide	5.80	m	CH	propylene
1.06	t, 7	CH ₃	ethanol	2.94	s	NCH ₃	dimethylacetamide	5.91	ddt	CHCH ₂	allyl acetate
1.09	t, 7	CH ₃	diethyl ether	3.16	s ⁹	CH ₃	methanol	5.93	ddt	CHCH ₂	diallyl carbonate
1.11	s	CH ₃	<i>tert</i> -butyl alcohol	3.24	s	OCH ₃	diglyme	6.01	m	CH(3,4)	pyrrole
1.15	br s	CH ₂	pump oil	3.24	s	CH ₃	1,2-dimethoxyethane	6.47	dd	CH(3,4)	furan
1.17	t, 7	CH ₂ CH ₃	ethyl acetate	3.33 ²	s	OH	water	6.52	s	OH ⁵	BHA
1.24	br s	CH ₂	H grease ⁸	3.34	s	CH ₂	ethylene glycol	6.62	s	ArH	BHA
1.25	m	CH ₂	<i>n</i> -hexane	3.38	q, 7	CH ₂	diethyl ether	6.65	s	OH ⁵	BHT
1.27	m	CH ₂	<i>n</i> -pentane	3.38	m	CH ₂	diglyme	6.73	m	CH(2,5)	pyrrole
1.29	sept, 7,3	CH ₂	propane	3.43	s	CH ₂	1,2-dimethoxyethane	6.87	s	ArH	BHT
1.36	s	ArC(CH ₃) ₃	BHA	3.44	q, 7 ⁹	CH ₂	ethanol	7.01	s	CH(4,5)	imidazole
1.36	s	ArC(CH ₃) ₃	BHT	3.51	s	CH ₂	18-crown-6	7.18	m	CH(2,4,6)	toluene
1.40	s	CH ₂	cyclohexane	3.51	m	CH ₂	diglyme	7.25	m	CH(3,5)	toluene
1.55	m	CH ₂ (3,4)	pyrrolidine	3.53	s	CH ₂	dimethyl malonate	7.37	s	CH	benzene
1.64-1.66	m	CH ₂ (4)	cyclohexanone	3.57	s	CH ₂	1,4-dioxane	7.39	m	CH(3,5)	pyridine
1.68	dt, 6,4, 1,5	CH ₃	propylene	3.60	m	CH ₂ (2,5)	tetrahydrofuran	7.61-7.67	m	CH(3,5)	benzaldehyde
1.74-1.78	m	CH ₂ (3,5)	cyclohexanone	3.65	s	CH ₃	dimethyl malonate	7.63	s	CH(2)	imidazole
1.76	m	CH ₂ (3,4)	tetrahydrofuran	3.66	s	ArOCH ₃	BHA	7.67	dd	CH(2,5)	furan
1.91	s	CH ₃	acetic acid	3.69	s	CH ₃	dimethyl carbonate	7.69-7.75	m	CH(4)	benzaldehyde
1.96	s	CH ₃ CO	dimethylacetamide	3.78	sept, 6	CH	2-propanol	7.79	m	CH(4)	pyridine
1.99	s	CH ₃ CO	ethyl acetate	3.90	s	CH ₂	1,2-dichloroethane	7.91-7.93	m	CH(2,6)	benzaldehyde
2.03	s	CH ₃	allyl acetate	4.01	s ⁹	OH	methanol	8.32	s	CH	chloroform
2.07	s	CH ₃	acetonitrile	4.03	q, 7	CH ₂ CH ₃	ethyl acetate	8.58	m	CH(2,6)	pyridine
2.07	s	CH ₃ CO	ethyl methyl ketone	4.19	s	OH	<i>tert</i> -butyl alcohol	10.02	s	HCO	benzaldehyde
2.09	s	CH ₃	acetone	4.42	s	CH ₃	nitromethane	10.75	br t	NH	pyrrole
2.14	s	CH ₃	hexamethylbenzene	4.52	ddd	CH ₂	allyl acetate				

Table S18. (CD₃)₂SO (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.01	CH ₄	methane	30.38	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	63.28	CH ₃	nitromethane	129.10	CH(3,5)	benzaldehyde
1.03	CH ₃	acetonitrile	30.56	CH ₃	acetone	64.32	CH ₂	allyl acetate	129.45	CH(2,6)	benzaldehyde
1.96	CH ₃	hexamethyldisiloxane	30.73	CH ₃	dimethylformamide	64.92	CH	2-propanol	131.10	C	hexamethylbenzene
6.61	CH ₃	ethane	30.95	CH ₂ (3,4)	<i>n</i> -hexane	66.36	CH ₂	1,4-dioxane	132.18	CHCH ₂	diallyl carbonate
7.61	CH ₂ CH ₃	ethyl methyl ketone	31.25	(CH ₃) ₃ C	BHT	66.88	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	132.71	CHCH ₂	allyl acetate
11.74	CH ₃	triethylamine	33.48	CH ₂ (3)	<i>n</i> -pentane	67.03	CH ₂ (2,5)	tetrahydrofuran	133.55	CH	propylene
13.28	CH ₃	<i>n</i> -pentane	34.33	(CH ₃) ₃ C	BHT	67.86	CH ₂	diallyl carbonate	134.52	CH(4)	benzaldehyde
13.88	CH ₃	<i>n</i> -hexane	34.42	NCH ₃	dimethylacetamide	69.54	CH ₂	diglyme	135.15	CH(2)	imidazole
14.40	CH ₃	ethyl acetate	34.76	(CH ₃) ₃ C	BHA	69.85	CH ₂	18-crown-6	136.05	CH(4)	pyridine
15.12	CH ₃	diethyl ether	35.73	CH ₃	dimethylformamide	71.17	CH ₂	1,2-dimethoxyethane	136.20	C(1)	benzaldehyde
15.67	CH ₂	propane	35.83	CH ₂ CH ₃	ethyl methyl ketone	71.25	CH ₂	diglyme	137.35	C(1)	toluene
16.34	CH ₃	propane	36.42 (d)	CH ₃	HMPA ¹¹	79.16	CH	chloroform	139.12	C(2,6)	BHT
16.60	CH ₃	hexamethylbenzene	37.38	NCH ₃	dimethylacetamide	95.44	CCl ₄	carbon tetrachloride	141.16	C(4)	BHA
18.51	CH ₃	ethanol	39.52 (sept)	CD ₃	(CD ₃) ₂ SO signal	107.07	CH(3,4)	pyrrole	142.82	CH(2,5)	furan
19.20	CH ₃	propylene	40.45	CH ₃	dimethyl sulfoxide	109.62	CH(3,4)	furan	147.44	C(2,6)	BHA
20.54	CH ₃	allyl acetate	40.72	CH ₂	dimethyl malonate	109.80	CH(3,5)	BHA	149.58	CH(2,6)	pyridine
20.68	CH ₃ CO	ethyl acetate	41.32	CH ₂ (2,6)	cyclohexanone	116.07	CH ₂	propylene	151.47	C(1)	BHT
20.95	CH ₃	acetic acid	45.02	CH ₂	1,2-dichloroethane	117.32	CH(2,5)	pyrrole	152.53	C(1)	BHA
20.97	CH ₂ Ar	BHT	45.74	CH ₂	triethylamine	117.64	CHCH ₂	allyl acetate	154.16	CO	diallyl carbonate
20.99	CH ₃	toluene	46.51	CH ₂ (2,5)	pyrrolidine	117.91	CN	acetonitrile	155.76	CO	dimethyl carbonate
21.29	CH ₃	dimethylacetamide	48.59	CH ₃	methanol	118.32	CHCH ₂	diallyl carbonate	162.29	CH	dimethylformamide
21.70	CH ₂ (2,4)	<i>n</i> -pentane	52.08	CH ₃	dimethyl malonate	121.55	CH(4,5)	imidazole	166.91	CO ₂	dimethyl malonate
22.05	CH ₂ (2,5)	<i>n</i> -hexane	54.63	CH ₃	dimethyl carbonate	123.52	CH ₂	ethylene	169.54	CO	dimethylacetamide
24.32	CH ₂ (4)	cyclohexanone	54.84	CH ₂	dichloromethane	123.84	CH(3,5)	pyridine	169.97	CO	allyl acetate
25.14	CH ₂ (3,4)	tetrahydrofuran	54.89	CH ₃ O	BHA	124.21	CO ₂	carbon dioxide	170.31	CO	ethyl acetate
25.26	CH ₂ (3,4)	pyrrolidine	56.07	CH ₂	ethanol	124.85	CH(3,5)	BHT	171.93	CO	acetic acid
25.43	CH ₃	2-propanol	57.98	CH ₃	diglyme	125.29	CH(4)	toluene	192.63	CS ₂	carbon disulfide
26.33	CH ₂	cyclohexane	58.03	CH ₃	1,2-dimethoxyethane	127.97	C(4)	BHT	193.08	HCO	benzaldehyde
26.46	CH ₂ (3,5)	cyclohexanone	59.74	CH ₂	ethyl acetate	128.18	CH(3,5)	toluene	206.31	CO	acetone
29.26	CH ₃ CO	ethyl methyl ketone	62.05	CH ₂	diethyl ether	128.30	CH	benzene	208.72	CO	ethyl methyl ketone
29.33	CH ₂	pump oil	62.76	CH ₂	ethylene glycol	128.88	CH(2,6)	toluene	210.63	CO	cyclohexanone
30.30	(CH ₃) ₃ C	BHA									

Table S19. CD₃CN (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.07	s	CH ₃	hexamethyldisiloxane	2.18	s	OH	<i>tert</i> -butyl alcohol	4.57	s	H ₂	hydrogen
0.08	s	CH ₃	silicone grease	2.19	s	CH ₃	hexamethylbenzene	4.61	ddd	CH ₂	diallyl carbonate
0.20	s	CH ₄	methane	2.22	s	ArCH ₃	BHT	4.93	dm, 10	CH ₂ (1)	propylene
0.85	s	CH ₃	ethane	2.27	t	CH ₂ (2,6)	cyclohexanone	4.98	s	OH ⁵	BHA
0.85	m	CH ₃	pump oil	2.33	s	CH ₃	toluene	5.04	dm, 17	CH ₂ (2)	propylene
0.89	t, 7	CH ₃	<i>n</i> -hexane	2.43	q, 7	CH ₂ CH ₃	ethyl methyl ketone	5.20	s	OH ⁵	BHT
0.89	t, 7	CH ₃	<i>n</i> -pentane	2.45	q, 7	CH ₂	triethylamine	5.21	ddt	CHCH ₂ (2)	allyl acetate
0.90	t, 7, 3	CH ₃	propane	2.47	s ^o	OH	ethanol	5.25	ddt	CHCH ₂ (2)	diallyl carbonate
0.96	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.50	s	CH ₃	dimethyl sulfoxide	5.29	ddt	CHCH ₂ (1)	allyl acetate
0.96	t, 7	CH ₃	triethylamine	2.57	d, 9, 5	CH ₃	HMPA	5.34	ddt	CHCH ₂ (1)	diallyl carbonate
1.09	d, 6	CH ₃	2-propanol	2.69 ⁷	m ⁷	OH ⁷	ethylene glycol ⁷	5.41	s	CH ₂	ethylene
1.12	t, 7	CH ₃	diethyl ether	2.75	m	CH ₂ (2,5)	pyrrolidine	5.44	s	CH	dichloromethane
1.12	t, 7	CH ₃	ethanol	2.77	s	CH ₃	dimethylformamide	5.85	m	CH	propylene
1.16	s	CH ₃	<i>tert</i> -butyl alcohol	2.83	s	NCH ₃	dimethylacetamide	5.93	ddt	CHCH ₂	allyl acetate
1.20	t, 7	CH ₂ CH ₃	ethyl acetate	2.89	s	CH ₃	dimethylformamide	5.96	ddt	CHCH ₂	diallyl carbonate
1.27	br s	CH ₂	pump oil	2.96	s	NCH ₃	dimethylacetamide	6.10	m	CH(3,4)	pyrrole
1.28	m	CH ₂	<i>n</i> -hexane	3.28	s	CH ₃	1,2-dimethoxyethane	6.44	dd	CH(3,4)	furan
1.29	m	CH ₂	<i>n</i> -pentane	3.28	s ^o	CH ₃	methanol	6.73	s	ArH	BHA
1.33	sept, 7, 3	CH ₂	propane	3.29	s	OCH ₃	diglyme	6.75	m	CH(2,5)	pyrrole
1.39	s	ArC(CH ₃) ₃	BHT	3.38	s	CH ₂	dimethyl malonate	6.97	s	ArH	BHT
1.40	s	ArC(CH ₃) ₃	BHA	3.42	q, 7	CH ₂	diethyl ether	7.01	s	CH(4,5)	imidazole
1.44	s	CH ₂	cyclohexane	3.45	m	CH ₂	diglyme	7.10-7.30	m	CH(2,4,6)	toluene
1.61	m	CH ₂ (3,4)	pyrrolidine	3.45	s	CH ₂	1,2-dimethoxyethane	7.10-7.30	m	CH(3,5)	toluene
1.67-1.72	m	CH ₂ (4)	cyclohexanone	3.51	s	CH ₂	18-crown-6	7.33	m	CH(3,5)	pyridine
1.70	dt, 6, 4, 1, 5	CH ₃	propylene	3.51	m ⁷	CH ₂	ethylene glycol	7.37	s	CH	benzene
1.79-1.84	m	CH ₂ (3,5)	cyclohexanone	3.53	m	CH ₂	diglyme	7.52	dd	CH(2,5)	furan
1.80	m	CH ₂ (3,4)	tetrahydrofuran	3.54	q, 7 ^o	CH ₂	ethanol	7.57	s	CH(2)	imidazole
1.94	p	CHD ₂	CD ₃ CN residual	3.60	s	CH ₂	1,4-dioxane	7.57-7.61	m	CH(3,5)	benzaldehyde
1.96	s	CH ₃	acetic acid	3.64	m	CH ₂ (2,5)	tetrahydrofuran	7.58	s	CH	chloroform
1.96	s	CH ₃	acetonitrile	3.68	s	CH ₃	dimethyl malonate	7.67-7.71	m	CH(4)	benzaldehyde
1.97	s	CH ₃ CO	dimethylacetamide	3.72	s	ArOCH ₃	BHA	7.73	m	CH(4)	pyridine
1.97	s	CH ₃ CO	ethyl acetate	3.72	s	CH ₃	dimethyl carbonate	7.89-7.91	m	CH(2,6)	benzaldehyde
2.02	s	CH ₃	allyl acetate	3.81	s	CH ₂	1,2-dichloroethane	7.92	s	CH	dimethylformamide
2.06	s	CH ₃ CO	ethyl methyl ketone	3.87	sept, 6	CH	2-propanol	8.57	m	CH(2,6)	pyridine
2.08	s	CH ₃	acetone	4.06	q, 7	CH ₂ CH ₃	ethyl acetate	9.27	br t	NH	pyrrole
2.13	s	OH	water	4.31	s	CH ₃	nitromethane	10.01	s	HCO	benzaldehyde
2.16	s ^o	OH	methanol	4.53	ddd	CH ₂	allyl acetate				

Table S20. CD₃CN (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.61	CH ₄	methane	30.68	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	65.55	CH ₂	allyl acetate	130.07	CH(3,5)	benzaldehyde
1.32 (sept)	CD ₃	CD ₃ CN signal	30.86	CH ₂	pump oil	66.32	CH ₂	diethyl ether	130.42	CH(2,6)	benzaldehyde
1.79	CH ₃	acetonitrile	30.91	CH ₃	acetone	67.72	CH ₂	1,4-dioxane	132.61	C	hexamethylbenzene
2.07	CH ₃	hexamethyldisiloxane	31.32	CH ₃	dimethylformamide	68.33	CH ₂ (2,5)	tetrahydrofuran	133.20	CHCH ₂	diallyl carbonate
6.99	CH ₃	ethane	31.50	(CH ₃) ₃ C	BHT	68.74	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	133.83	CHCH ₂	allyl acetate
8.14	CH ₂ CH ₃	ethyl methyl ketone	32.36	CH ₂ (3,4)	<i>n</i> -hexane	69.09	CH ₂	diallyl carbonate	134.78	CH	propylene
12.38	CH ₃	triethylamine	34.89	CH ₂ (3)	<i>n</i> -pentane	70.99	CH ₂	diglyme	135.40	CH(4)	benzaldehyde
14.37	CH ₃	<i>n</i> -pentane	35.05	(CH ₃) ₃ C	BHT	71.22	CH ₂	18-crown-6	136.33	CH(2)	imidazole
14.43	CH ₃	<i>n</i> -hexane	35.17	NCH ₃	dimethylacetamide	72.47	CH ₂	1,2-dimethoxyethane	136.89	CH(4)	pyridine
14.54	CH ₃	ethyl acetate	35.48	(CH ₃) ₂ C	BHA	72.63	CH ₂	diglyme	137.62	C(1)	benzaldehyde
15.63	CH ₃	diethyl ether	36.57	CH ₃	dimethylformamide	79.17	CH	chloroform	138.13	C(2,6)	BHT
16.73	CH ₃	propane	37.09	CH ₂ CH ₃	ethyl methyl ketone	96.68	CCl ₄	carbon tetrachloride	138.90	C(1)	toluene
16.91	CH ₂	propane	37.10 (d)	CH ₃	HMPA ¹¹	108.31	CH(3,4)	pyrrole	140.20	C(4)	BHA
16.94	CH ₃	hexamethylbenzene	38.26	NCH ₃	dimethylacetamide	110.49	CH(3,4)	furan	143.74	CH(2,5)	furan
18.80	CH ₃	ethanol	41.31	CH ₃	dimethyl sulfoxide	111.35	CH(3,5)	BHA	148.39	C(2,6)	BHA
19.48	CH ₃	propylene	41.77	CH ₂	dimethyl malonate	116.12	CH ₂	propylene	150.76	CH(2,6)	pyridine
20.73	CH ₃	acetic acid	42.44	CH ₂ (2,6)	cyclohexanone	118.06	CHCH ₂	allyl acetate	152.42	C(1)	BHT
21.02	CH ₃	allyl acetate	45.54	CH ₂	1,2-dichloroethane	118.26	CN	CD ₃ CN signal	154.02	C(1)	BHA
21.16	CH ₃ CO	ethyl acetate	47.10	CH ₂	triethylamine	118.26	CN	acetonitrile	155.66	CO	diallyl carbonate
21.23	CH ₃ Ar	BHT	47.57	CH ₂ (2,5)	pyrrolidine	118.47	CH(2,5)	pyrrole	157.26	CO	dimethyl carbonate
21.50	CH ₃	toluene	49.90	CH ₃	methanol	118.86	CHCH ₂	diallyl carbonate	163.31	CH	dimethylformamide
21.76	CH ₃	dimethylacetamide	52.95	CH ₃	dimethyl malonate	122.78	CH(4,5)	imidazole	168.07	CO ₂	dimethyl malonate
23.08	CH ₂ (2,4)	<i>n</i> -pentane	55.32	CH ₂	dichloromethane	123.69	CH ₂	ethylene	171.31	CO	dimethylacetamide
23.40	CH ₂ (2,5)	<i>n</i> -hexane	55.39	CH ₃	dimethyl carbonate	125.89	CO ₂	carbon dioxide	171.32	CO	allyl acetate
25.55	CH ₃	2-propanol	55.94	CH ₃ O	BHA	126.28	CH(4)	toluene	171.68	CO	ethyl acetate
25.62	CH ₂ (4)	cyclohexanone	57.96	CH ₂	ethanol	126.38	CH(3,5)	BHT	173.21	CO	acetic acid
26.27	CH ₂ (3,4)	tetrahydrofuran	58.89	CH ₃	1,2-dimethoxyethane	127.76	CH(3,5)	pyridine	193.60	CS ₂	carbon disulfide
26.34	CH ₂ (3,4)	pyrrolidine	58.90	CH ₃	diglyme	129.23	CH(3,5)	toluene	193.64	HCO	benzaldehyde
27.63	CH ₂	cyclohexane	60.98	CH ₂	ethyl acetate	129.32	CH	benzene	207.43	CO	acetone
27.80	CH ₂ (3,5)	cyclohexanone	63.66	CH ₃	nitromethane	129.61	C(4)	BHT	209.88	CO	ethyl methyl ketone
29.60	CH ₃ CO	ethyl methyl ketone	64.22	CH ₂	ethylene glycol	129.94	CH(2,6)	toluene	211.99	CO	cyclohexanone
30.55	(CH ₃) ₃ C	BHA	64.30	CH	2-propanol						

Table S21. TFE- d_3 (^1H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.08	s	CH ₃	hexamethyldisiloxane	2.20	s	OH	<i>tert</i> -butyl alcohol	4.53	s	H ₂	hydrogen
0.16	s	CH ₃	silicone grease	2.24	s	ArCH ₃	BHT	4.58	ddd	CH ₂	allyl acetate
0.18	s	CH ₄	methane	2.24	s	CH ₃	hexamethylbenzene	4.62	ddd	CH ₂	diallyl carbonate
0.85	s	CH ₃	ethane	2.33	s	CH ₃	toluene	4.93	dm, 10	CH ₂ (1)	propylene
0.88-0.94	m	CH ₃	H grease ^δ	2.38	t	CH ₂ (2,6)	cyclohexanone	5.02	s	OH	TFE- d_3 residual
0.90	t, 7	CH ₃	<i>n</i> -pentane	2.49	q, 7	CH ₂ CH ₃	ethyl methyl ketone	5.03	dm, 17	CH ₂ (2)	propylene
0.90	t, 7.3	CH ₃	propane	2.63	s	CH ₃	dimethyl sulfoxide	5.24	s	CH ₂	dichloromethane
0.91	t, 7	CH ₃	<i>n</i> -hexane	2.63	d, 9.5	CH ₃	HMPA	5.25	ddt	CHCH ₂ (2)	allyl acetate
0.99	m	CH ₃	pump oil	2.88	s	CH ₃	dimethylformamide	5.28	ddt	CHCH ₂ (2)	diallyl carbonate
1.05	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.94	s	NCH ₃	dimethylacetamide	5.32	ddt	CHCH ₂ (1)	allyl acetate
1.20	t, 7	CH ₃	diethyl ether	2.98	s	CH ₃	dimethylformamide	5.35	ddt	CHCH ₂ (1)	diallyl carbonate
1.20	d, 6	CH ₃	2-propanol	3.05	s	NCH ₃	dimethylacetamide	5.40	s	CH ₂	ethylene
1.22	t, 7	CH ₃	ethanol	3.11	m	CH ₂ (2,5)	pyrrolidine	5.87	m	CH	propylene
1.26	t, 7	CH ₂ CH ₃	ethyl acetate	3.12	q, 7	CH ₂	triethylamine	5.92	ddt	CHCH ₂	diallyl carbonate
1.28	s	CH ₃	<i>tert</i> -butyl alcohol	3.40	s	CH ₃	1,2-dimethoxyethane	5.93	ddt	CHCH ₂	allyl acetate
1.31	m	CH ₂	<i>n</i> -hexane	3.41	s	OCH ₃	diglyme	6.24	m	CH(3,4)	pyrrole
1.31	t, 7	CH ₃	triethylamine	3.41	s	CH ₂	dimethyl malonate	6.42	dd	CH(3,4)	furane
1.33	br s	CH ₂	H grease ^δ	3.44	s	CH ₃	methanol	6.84	m	CH(2,5)	pyrrole
1.33	m	CH ₂	<i>n</i> -pentane	3.58	q, 7	CH ₂	diethyl ether	6.87	s	ArH	BHA
1.33	sept, 7.3	CH ₂	propane	3.61	s	CH ₂	1,2-dimethoxyethane	7.03	s	CH(4,5)	imidazole
1.41	br s	CH ₂	pump oil	3.62	m	CH ₂	diglyme	7.06	s	ArH	BHT
1.43	s	ArC(CH ₃) ₃	BHT	3.64	s	CH ₂	18-crown-6	7.10-7.30	m	CH(2,4,6)	toluene
1.44	s	ArC(CH ₃) ₃	BHA	3.66	s	OH	water	7.10-7.30	m	CH(3,5)	toluene
1.47	s	CH ₂	cyclohexane	3.67	m	CH ₂	diglyme	7.33	s	CH	chloroform
1.70	dt, 6.4, 1.5	CH ₃	propylene	3.71	s	CH ₂	1,2-dichloroethane	7.36	s	CH	benzene
1.75-1.78	m	CH ₂ (4)	cyclohexanone	3.71	q, 7	CH ₂	ethanol	7.40	dd	CH(3,5)	pyridine
1.87-1.92	m	CH ₂ (3,5)	cyclohexanone	3.72	s	CH ₂	ethylene glycol	7.44	dd	CH(2,5)	furane
1.91	m	CH ₂ (3,4)	tetrahydrofuran	3.76	s	CH ₃	dimethyl malonate	7.56-7.59	m	CH(3,5)	benzaldehyde
1.93	m	CH ₂ (3,4)	pyrrolidine	3.76	s	CH ₂	1,4-dioxane	7.61	s	CH(2)	imidazole
1.95	s	CH ₃	acetonitrile	3.77	s	CH ₃	dimethyl carbonate	7.68-7.72	m	CH(4)	benzaldehyde
2.03	s	CH ₃ CO	ethyl acetate	3.78	m	CH ₂ (2,5)	tetrahydrofuran	7.82	m	CH(4)	pyridine
2.06	s	CH ₃	acetic acid	3.79	s	ArOCH ₃	BHA	7.86	s	CH	dimethylformamide
2.07	s	CH ₃	allyl acetate	3.88	tq	CDH	TFE- d_3 residual	7.90-7.92	m	CH(2,6)	benzaldehyde
2.09	s	CH ₃ CO	dimethylacetamide	4.05	sept, 6	CH	2-propanol	8.45	m	CH(2,6)	pyridine
2.16	s	CH ₃ CO	ethyl methyl ketone	4.14	q, 7	CH ₂ CH ₃	ethyl acetate	9.88	s	HCO	benzaldehyde
2.19	s	CH ₃	acetone	4.28	s	CH ₃	nitromethane				

Table S22. TFE- d_3 ($^{13}\text{C}\{^1\text{H}\}$ NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-5.88	CH ₄	methane	30.96	CH ₃	dimethylformamide	66.69	CH	2-propanol	130.82	CH(3,5)	benzaldehyde
1.00	CH ₃	acetonitrile	31.01	(CH ₃) ₂ C	BHT	67.55	CH ₂	diethyl ether	131.78	CH(2,6)	benzaldehyde
2.09	CH ₃	hexamethyldisiloxane	31.07	(CH ₃) ₂ C	<i>tert</i> -butyl alcohol	67.61	CH ₂	allyl acetate	132.72	CHCH ₂	diallyl carbonate
2.87	CH ₃	silicone grease	31.85	CH ₂	pump oil	68.52	CH ₃	1,4-dioxane	133.33	CHCH ₂	allyl acetate
7.01	CH ₃	ethane	32.35	CO	acetone	69.53	CH ₂ (2,5)	tetrahydrofuran	134.04	C	hexamethylbenzene
8.29	CH ₂ CH ₃	ethyl methyl ketone	33.17	CH ₂ (3,4)	<i>n</i> -hexane	70.69	CH ₂	diallyl carbonate	136.00	CH	propylene
9.51	CH ₃	triethylamine	35.69	(CH ₃) ₂ C	BHT	70.80	CH ₂	18-crown-6	136.58	CH(2)	imidazole
14.36	CH ₃	ethyl acetate	35.76	CH ₂ (3)	<i>n</i> -pentane	71.33	CH ₂	diglyme	137.17	CH(4)	benzaldehyde
14.54	CH ₃	<i>n</i> -pentane	36.07	(CH ₃) ₂ C	BHA	72.35	(CH ₃) ₂ C	<i>tert</i> -butyl alcohol	137.84	C(1)	benzaldehyde
14.63	CH ₃	<i>n</i> -hexane	36.28	NCH ₃	dimethylacetamide	72.87	CH ₂	1,2-dimethoxyethane	138.59	C(2,6)	BHT
15.33	CH ₃	diethyl ether	37.21 (d)	CH ₃	HMPA	73.05	CH ₂	diglyme	139.62	CH(4)	pyridine
16.93	CH ₃	propane	37.76	CH ₃	dimethylformamide	78.83	CH	chloroform	139.92	C(1)	toluene
17.04	CH ₃	hexamethylbenzene	38.23	CH ₂ CH ₃	ethyl methyl ketone	97.74	CCl ₄	carbon tetrachloride	140.23	C(4)	BHA
17.46	CH ₂	propane	39.06	NCH ₃	dimethylacetamide	108.85	CH(3,4)	pyrrole	144.22	CH(2,5)	furane
18.11	CH ₂	ethanol	40.06	CH ₃	dimethyl sulfoxide	111.06	CH(3,4)	furane	149.76	CH(2,6)	pyridine
19.63	CH ₃	propylene	42.13	CH ₂	dimethyl malonate	112.90	CH(3,5)	BHA	150.52	C(2,6)	BHA
20.91	CH ₃	acetic acid	43.16	CH ₂ (2,6)	cyclohexanone	116.38	CH ₂	propylene	153.46	C(1)	BHT
21.10	CH ₃	allyl acetate	45.28	CH ₂	1,2-dichloroethane	118.95	CN	acetonitrile	153.74	C(1)	BHA
21.18	CH ₃ CO	ethyl acetate	47.43	CH ₂ (2,5)	pyrrolidine	119.39	CHCH ₂	allyl acetate	157.39	CO	diallyl carbonate
21.34	CH ₃ Ar	BHT	48.45	CH ₂	triethylamine	119.61	CH(2,5)	pyrrole	159.04	CO	dimethyl carbonate
21.40	CH ₃	dimethylacetamide	50.67	CH ₃	methanol	120.15	CHCH ₂	diallyl carbonate	166.01	CH	dimethylformamide
21.62	CH ₃	toluene	54.00	CH ₃	dimethyl malonate	122.93	CH(4,5)	imidazole	170.88	CO ₂	dimethyl malonate
23.75	CH ₂ (2,4)	<i>n</i> -pentane	54.46	CH ₂	dichloromethane	124.08	CH ₂	ethylene	175.55	CO	ethyl acetate
24.06	CH ₂ (2,5)	<i>n</i> -hexane	56.17	CH ₃	dimethyl carbonate	126.27	CH(3,5)	pyridine	175.74	CO	dimethylacetamide
25.21	CH ₃	2-propanol	57.55	CH ₃ O	BHA	126.28 (q)	CF ₃	TFE- d_3 signal	175.98	CO	allyl acetate
25.73	CH ₂ (3,4)	pyrrolidine	59.40	CH ₃	diglyme	126.82	CH(4)	toluene	177.96	CO	acetic acid
26.00	CH ₂ (4)	cyclohexanone	59.52	CH ₃	1,2-dimethoxyethane	126.92	CO ₂	carbon dioxide	196.26	CS ₂	carbon disulfide
26.69	CH ₂ (3,4)	tetrahydrofuran	59.68	CH ₂	ethanol	127.11	CH(3,5)	BHT	197.63	HCO	benzaldehyde
28.34	CH ₂	cyclohexane	61.5 (qp)	CD ₂	TFE- d_3 signal	129.79	CH(3,5)	toluene	214.98	CH ₃	acetone
28.56	CH ₂ (3,5)	cyclohexanone	62.70	CH ₂	ethyl acetate	129.84	CH	benzene	218.31	CO	ethyl methyl ketone
29.64	CH ₃ CO	ethyl methyl ketone	63.17	CH ₃	nitromethane	130.58	CH(2,6)	toluene	221.30	CO	cyclohexanone
30.80	(CH ₃) ₂ C	BHA	64.87	CH ₂	ethylene glycol	130.62	C(4)	BHT			

Table S23. CD₃OD (¹H NMR data by chemical shift in ppm)

shift	mult	proton	impurity	shift	mult	proton	impurity	shift	mult	proton	impurity
0.07	s	CH ₃	hexamethyldisiloxane	2.19	s	CH ₃	hexamethylbenzene	4.56	s	H ₂	hydrogen
0.10	s	CH ₃	silicone grease	2.21	s	ArCH ₃	BHT	4.61	ddd	CH ₂	diallyl carbonate
0.20	s	CH ₄	methane	2.32	s	CH ₃	toluene	4.85	s	OH ^d	BHA
0.85	s	CH ₃	ethane	2.34	t	CH ₂ (2,6)	cyclohexanone	4.87	s	OH	water
0.86-0.91	m	CH ₃	pump oil	2.50	q, 7	CH ₂ CH ₃	ethyl methyl ketone	4.91	dm, 10	CH ₂ (1)	propylene
0.86-0.93	m	CH ₃	H grease ⁸	2.58	q, 7	CH ₂	triethylamine	5.01	dm, 17	CH ₂ (2)	propylene
0.90	t, 7	CH ₃	<i>n</i> -hexane	2.64	d, 9,5	CH ₃	HMPA	5.21	ddt	CHCH ₂ (2)	allyl acetate
0.90	t, 7	CH ₃	<i>n</i> -pentane	2.65	s	CH ₃	dimethyl sulfoxide	5.25	ddt	CHCH ₂ (2)	diallyl carbonate
0.91	t, 7,3	CH ₃	propane	2.80	m	CH ₂ (2,5)	pyrrolidine	5.30	ddt	CHCH ₂ (1)	allyl acetate
1.01	t, 7	CH ₂ CH ₃	ethyl methyl ketone	2.86	s	CH ₃	dimethylformamide	5.34	ddt	CHCH ₂ (1)	diallyl carbonate
1.05	t, 7	CH ₃	triethylamine	2.92	s	NCH ₃	dimethylacetamide	5.39	s	CH ₂	ethylene
1.15	d, 6	CH ₃	2-propanol	2.99	s	CH ₃	dimethylformamide	5.49	s	CH ₂	dichloromethane
1.18	t, 7	CH ₃	diethyl ether	3.31	p	CD ₂ H	CD ₃ OD residual	5.82	m	CH	propylene
1.19	t, 7	CH ₃	ethanol	3.31	s	NCH ₃	dimethylacetamide	5.94	ddt	CHCH ₂	allyl acetate
1.24	t, 7	CH ₂ CH ₃	ethyl acetate	3.34	s	CH ₃	methanol	5.94	ddt	CHCH ₂	diallyl carbonate
1.29	br s	CH ₂	H grease ⁸	3.35	s	OCH ₃	diglyme	6.08	m	CH(3,4)	pyrrole
1.29	m	CH ₂	<i>n</i> -hexane	3.35	s	CH ₃	1,2-dimethoxyethane	6.40	dd	CH(3,4)	furan
1.29	br s	CH ₂	<i>n</i> -pentane	3.44	s	CH ₂	dimethyl malonate	6.71	s	ArH	BHA
1.29	1.34	CH ₂	pump oil	3.49	q, 7	CH ₂	diethyl ether	6.72	m	CH(2,5)	pyrrole
1.40	sept, 7,3	CH ₂	propane	3.52	s	CH ₂	1,2-dimethoxyethane	6.92	s	ArH	BHT
1.40	s	CH ₃	<i>tert</i> -butyl alcohol	3.58	m	CH ₂	diglyme	7.05	s	CH(4,5)	imidazole
1.40	s	ArC(CH ₃) ₃	BHT	3.59	s	CH ₂	ethylene glycol	7.16	m	CH(2,4,6)	toluene
1.41	s	ArC(CH ₃) ₃	BHA	3.60	q, 7	CH ₂	ethanol	7.16	m	CH(3,5)	toluene
1.45	s	CH ₂	cyclohexane	3.61	m	CH ₂	diglyme	7.33	s	CH	benzene
1.70	dt, 6,4, 1,5	CH ₃	propylene	3.64	s	CH ₂	18-crown-6	7.44	m	CH(3,5)	pyridine
1.72	m	CH ₂ (3,4)	pyrrolidine	3.66	s	CH ₂	1,4-dioxane	7.49	dd	CH(2,5)	furan
1.74-1.76	m	CH ₂ (4)	cyclohexanone	3.71	m	CH ₂ (2,5)	tetrahydrofuran	7.56-7.60	m	CH(3,5)	benzaldehyde
1.85-1.87	m	CH ₂ (3,5)	cyclohexanone	3.72	s	ArOCH ₃	BHA	7.66-7.70	m	CH(4)	benzaldehyde
1.87	m	CH ₂ (3,4)	tetrahydrofuran	3.72	s	CH ₃	dimethyl malonate	7.67	s	CH(2)	imidazole
1.99	s	CH ₃	acetic acid	3.74	s	CH ₃	dimethyl carbonate	7.85	m	CH(4)	pyridine
2.01	s	CH ₃ CO	ethyl acetate	3.78	s	CH ₂	1,2-dichloroethane	7.90	s	CH	chloroform
2.03	s	CH ₃	acetonitrile	3.92	sept, 6	CH	2-propanol	7.90-7.93	m	CH(2,6)	benzaldehyde
2.05	s	CH ₃	allyl acetate	4.09	q, 7	CH ₂ CH ₃	ethyl acetate	7.97	s	CH	dimethylformamide
2.07	s	CH ₃ CO	dimethylacetamide	4.34	s	CH ₃	nitromethane	8.53	m	CH(2,6)	pyridine
2.12	s	CH ₃ CO	ethyl methyl ketone	4.56	ddd	CH ₂	allyl acetate	10.00	s	HCO	benzaldehyde
2.15	s	CH ₃	acetone								

Table S24. CD₃OD (¹³C{¹H} NMR data by chemical shift in ppm)

shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity	shift	carbon	impurity
-4.90	CH ₄	methane	30.82	(CH ₃) ₃ C	BHA	64.71	CH	2-propanol	130.12	CH(3,5)	benzaldehyde
0.85	CH ₃	acetonitrile	30.91	(CH ₃) ₃ C	<i>tert</i> -butyl alcohol	66.14	CH ₂	allyl acetate	130.64	CH(2,6)	benzaldehyde
1.99	CH ₃	hexamethyldisiloxane	31.15	(CH ₃) ₃ C	BHT	66.88	CH ₂	diethyl ether	132.53	C	hexamethylbenzene
2.10	CH ₃	silicone grease	31.35	CH ₂	pump oil	68.11	CH ₂	1,4-dioxane	133.25	CHCH ₂	diallyl carbonate
6.98	CH ₃	ethane	31.61	CH ₃	dimethylformamide	68.83	CH ₂ (2,5)	tetrahydrofuran	133.71	CHCH ₂	allyl acetate
8.09	CH ₂ CH ₃	ethyl methyl ketone	32.73	CH ₂ (3,4)	<i>n</i> -hexane	69.35	CH ₂	diallyl carbonate	134.61	CH	propylene
11.09	CH ₃	triethylamine	35.30	CH ₂ (3)	<i>n</i> -pentane	69.40	(CH ₃) ₂ C	<i>tert</i> -butyl alcohol	135.60	CH(4)	benzaldehyde
14.39	CH ₃	<i>n</i> -pentane	35.36	(CH ₃) ₃ C	BHT	71.33	CH ₂	diglyme	136.31	CH(2)	imidazole
14.45	CH ₃	<i>n</i> -hexane	35.50	NCH ₃	dimethylacetamide	71.47	CH ₂	18-crown-6	137.96	C(1)	benzaldehyde
14.49	CH ₃	ethyl acetate	35.83	(CH ₃) ₃ C	BHA	72.72	CH ₂	1,2-dimethoxyethane	138.35	CH(4)	pyridine
15.46	CH ₃	diethyl ether	36.89	CH ₃	dimethylformamide	72.92	CH ₂	diglyme	138.85	C(1)	toluene
16.80	CH ₃	propane	37.00 (d)	CH ₃	HMPA ¹	79.44	CH	chloroform	139.09	C(2,6)	BHT
16.90	CH ₃	hexamethylbenzene	37.34	CH ₂ CH ₃	ethyl methyl ketone	97.21	CCl ₄	carbon tetrachloride	141.36	C(4)	BHA
17.19	CH ₂	propane	38.43	NCH ₃	dimethylacetamide	108.11	CH(3,4)	pyrrole	143.68	CH(2,5)	furan
18.40	CH ₃	ethanol	40.45	CH ₃	dimethyl sulfoxide	110.33	CH(3,4)	furan	149.04	C(2,6)	BHA
19.50	CH ₃	propylene	41.60	CH ₂	dimethyl malonate	111.30	CH(3,5)	BHA	150.07	CH(2,6)	pyridine
20.56	CH ₃	acetic acid	42.61	CH ₂ (2,6)	cyclohexanone	116.04	CH ₂	propylene	152.85	C(1)	BHT
20.71	CH ₃	allyl acetate	45.11	CH ₂	1,2-dichloroethane	118.06	CN	acetonitrile	154.34	C(1)	BHA
20.88	CH ₃ CO	ethyl acetate	46.96	CH ₂	triethylamine	118.22	CHCH ₂	allyl acetate	156.28	CO	diallyl carbonate
21.32	CH ₃	dimethylacetamide	47.23	CH ₂ (2,5)	pyrrolidine	118.28	CH(2,5)	pyrrole	157.91	CO	dimethyl carbonate
21.38	CH ₃ Ar	BHT	49.00 (sept)	CD ₃	CD ₃ OD signal	118.74	CHCH ₂	diallyl carbonate	164.73	CH	dimethylformamide
21.50	CH ₃	toluene	49.86	CH ₃	methanol	122.60	CH(4,5)	imidazole	168.70	CO ₂	dimethyl malonate
23.38	CH ₂ (2,4)	<i>n</i> -pentane	52.83	CH ₃	dimethyl malonate	123.46	CH ₂	ethylene	172.41	CO	allyl acetate
23.68	CH ₂ (2,5)	<i>n</i> -hexane	54.78	CH ₂	dichloromethane	125.53	CH(3,5)	pyridine	172.89	CO	ethyl acetate
25.27	CH ₃	2-propanol	55.25	CH ₃	dimethyl carbonate	126.11	CH(3,5)	BHT	173.32	CO	dimethylacetamide
25.86	CH ₂ (4)	cyclohexanone	55.96	CH ₃ O	BHA	126.29	CH(4)	toluene	175.11	CO	acetic acid
26.29	CH ₂ (3,4)	pyrrolidine	58.26	CH ₂	ethanol	126.31	CO ₂	carbon dioxide	193.82	CS ₂	carbon disulfide
26.48	CH ₂ (3,4)	tetrahydrofuran	59.06	CH ₃	diglyme	129.20	CH(3,5)	toluene	194.11	HCO	benzaldehyde
27.96	CH ₂	cyclohexane	59.06	CH ₃	1,2-dimethoxyethane	129.34	CH	benzene	209.67	CO	acetone
28.16	CH ₂ (3,5)	cyclohexanone	61.50	CH ₂	ethyl acetate	129.49	CH	BHT	212.16	CO	ethyl methyl ketone
29.39	CH ₃ CO	ethyl methyl ketone	63.08	CH ₃	nitromethane	129.91	CH(2,6)	toluene	214.69	CO	cyclohexanone
30.67	CH ₃	acetone	64.30	CH ₂	ethylene glycol						

Table S25. D₂O (¹H NMR data by chemical shift in ppm)

<i>shift</i>	<i>mult</i>	<i>proton</i>	<i>impurity</i>	<i>shift</i>	<i>mult</i>	<i>proton</i>	<i>impurity</i>	<i>shift</i>	<i>mult</i>	<i>proton</i>	<i>impurity</i>
0.18	s	CH ₄	methane	2.71	s	CH ₃	dimethyl sulfoxide	4.69	ddd	CH ₂	diallyl carbonate
0.28	s	CH ₃	hexamethyldisiloxane	2.85	s	CH ₃	dimethylformamide	4.79	s	HOD	D ₂ O residual
0.82	s	CH ₃	ethane	2.90	s	NCH ₃	dimethylacetamide	4.95	dm, 10	CH ₂ (1)	propylene
0.88	t, 7.3	CH ₃	propane	3.01	s	CH ₃	dimethylformamide	5.06	dm, 17	CH ₂ (2)	propylene
0.99	t, 7	CH ₃	triethylamine	3.06	s	NCH ₃	dimethylacetamide	5.30	ddt	CHCH ₂ (2)	allyl acetate
1.17	t, 7	CH ₃	diethyl ether	3.07	m	CH ₂ (2,5)	pyrrolidine	5.32	ddt	CHCH ₂ (2)	diallyl carbonate
1.17	t, 7	CH ₃	ethanol	3.18	q, 7	CH ₂ CH ₃	ethyl methyl ketone	5.37	ddt	CHCH ₂ (1)	allyl acetate
1.17	d, 6	CH ₃	2-propanol	3.34	s	CH ₃	methanol	5.40	ddt	CHCH ₂ (1)	diallyl carbonate
1.24	s	CH ₃	tert-butyl alcohol	3.37	s	OCH ₃	diglyme	5.44	s	CH ₂	ethylene
1.24	t, 7	CH ₂ CH ₃	ethyl acetate	3.37	s	CH ₃	1,2-dimethoxyethane	5.90	m	CH	propylene
1.26	t, 7	CH ₂ CH ₃	ethyl methyl ketone	3.56	q, 7	CH ₂	diethyl ether	5.99	ddt	CHCH ₂	allyl acetate
1.30	sept, 7.3	CH ₂	propane	3.60	s	CH ₂	1,2-dimethoxyethane	5.99	ddt	CHCH ₂	diallyl carbonate
1.70	dt, 6.4, 1.5	CH ₃	propylene	3.60	s	CH ₂	dimethyl malonate	6.26	m	CH(3,4)	pyrrole
1.70-1.75	m	CH ₂ (4)	cyclohexanone	3.61	m	CH ₂	diglyme	6.51	dd	CH(3,4)	furan
1.85-1.90	m	CH ₂ (3,5)	cyclohexanone	3.65	q, 7	CH ₂	ethanol	6.93	m	CH(2,5)	pyrrole
1.87	m	CH ₂ (3,4)	pyrrolidine	3.65	s	CH ₂	ethylene glycol	7.14	s	CH(4,5)	imidazole
1.88	m	CH ₂ (3,4)	tetrahydrofuran	3.67	m	CH ₂	diglyme	7.45	m	CH(3,5)	pyridine
2.06	s	CH ₃	acetonitrile	3.69	s	CH ₃	dimethyl carbonate	7.57	dd	CH(2,5)	furan
2.07	s	CH ₂ CO	ethyl acetate	3.74	m	CH ₂ (2,5)	tetrahydrofuran	7.57-7.66	m	CH(3,5)	benzaldehyde
2.08	s	CH ₃	acetic acid	3.75	s	CH ₃	1,4-dioxane	7.76-7.80	m	CH(4)	benzaldehyde
2.08	s	CH ₂ CO	dimethylacetamide	3.78	s	CH ₃	dimethyl malonate	7.78	s	CH(2)	imidazole
2.13	s	CH ₃	allyl acetate	3.80	s	CH ₂	18-crown-6	7.87	m	CH(4)	pyridine
2.19	s	CH ₂ CO	ethyl methyl ketone	4.02	sept, 6	CH	2-propanol	7.92	s	CH	dimethylformamide
2.22	s	CH ₃	acetone	4.14	q, 7	CH ₂ CH ₃	ethyl acetate	7.97-7.99	m	CH(2,6)	benzaldehyde
2.40	t	CH ₂ (2,6)	cyclohexanone	4.40	s	CH ₃	nitromethane	8.52	m	CH(2,6)	pyridine
2.57	q, 7	CH ₂	triethylamine	4.62	ddd	CH ₂	allyl acetate	9.96	s	HCO	benzaldehyde
2.61	d, 9.5	CH ₃	HMPA								

Table S26. D₂O (¹³C{¹H} NMR data by chemical shift in ppm)

<i>shift</i>	<i>carbon</i>	<i>impurity</i>	<i>shift</i>	<i>carbon</i>	<i>impurity</i>	<i>shift</i>	<i>carbon</i>	<i>impurity</i>	<i>shift</i>	<i>carbon</i>	<i>impurity</i>
1.47	CH ₃	acetonitrile	36.46 (d)	CH ₃	HMPA'	67.19	CH ₂	1,4-dioxane	132.76	CHCH ₂	diallyl carbonate
2.31	CH ₃	hexamethyldisiloxane	37.27	CH ₂ CH ₃	ethyl methyl ketone	68.68	CH ₂ (2,5)	tetrahydrofuran	134.70	CH (4)	benzaldehyde
7.87	CH ₂ CH ₃	ethyl methyl ketone	37.54	CH ₃	dimethylformamide	68.81	CH ₂	diallyl carbonate	136.11	C(1)	benzaldehyde
9.07	CH ₃	triethylamine	38.76	NCH ₃	dimethylacetamide	70.05	CH ₂	diglyme	136.65	CH(2)	imidazole
13.92	CH ₃	ethyl acetate	39.39	CH ₃	dimethyl sulfoxide	70.14	CH ₂	18-crown-6	138.27	CH(4)	pyridine
14.77	CH ₃	diethyl ether	42.02	CH ₂ (2,6)	cyclohexanone	70.36	(CH ₃) ₃ C	tert-butyl alcohol	143.57	CH(2,5)	furan
17.47	CH ₃	ethanol	42.13	CH ₂	dimethyl malonate	71.49	CH ₂	1,2-dimethoxyethane	149.18	CH(2,6)	pyridine
21.00	CH ₃	allyl acetate	46.83	CH ₂ (2,5)	pyrrolidine	71.63	CH ₂	diglyme	157.78	CO	diallyl carbonate
21.03	CH ₃	acetic acid	47.19	CH ₂	triethylamine	96.73	CCl ₄	carbon tetrachloride	163.96	CO	dimethyl carbonate
21.09	CH ₃	dimethylacetamide	49.50 ¹²	CH ₃	methanol	107.83	CH(3,4)	pyrrole	165.53	CH	dimethylformamide
21.15	CH ₂ CO	ethyl acetate	53.65	CH ₃	dimethyl malonate	110.23	CH(3,4)	furan	170.12	CO ₂	dimethyl malonate
24.38	CH ₃	2-propanol	55.81	CH ₃	dimethyl carbonate	118.75	CHCH ₂	diallyl carbonate	174.57	CO	dimethylacetamide
24.77	CH ₂ (4)	cyclohexanone	58.05	CH ₂	ethanol	119.03	CHCH ₂	allyl acetate	174.78	CO	allyl acetate
25.67	CH ₂ (3,4)	tetrahydrofuran	58.67	CH ₃	diglyme	119.06	CH(2,5)	pyrrole	175.26	CO	ethyl acetate
25.86	CH ₂ (3,4)	pyrrolidine	58.67	CH ₃	1,2-dimethoxyethane	119.68	CN	acetonitrile	177.21	CO	acetic acid
27.50	CH ₂ (3,5)	cyclohexanone	62.32	CH ₂	ethyl acetate	122.43	CH(4,5)	imidazole	191.67	HCO	benzaldehyde
29.49	CH ₂ CO	ethyl methyl ketone	63.17	CH ₂	ethylene glycol	125.12	CH(3,5)	pyridine	197.25	CS ₂	carbon disulfide
30.29	(CH ₃) ₃ C	tert-butyl alcohol	63.22	CH ₃	nitromethane	129.48	CH(3,5)	benzaldehyde	215.94	CO	acetone
30.89	CH ₃	acetone	64.88	CH	2-propanol	130.09	CH(2,6)	benzaldehyde	218.43	CO	ethyl methyl ketone
32.03	CH ₃	dimethylformamide	66.42	CH ₂	diethyl ether	132.48	CHCH ₂	allyl acetate	221.22	CO	cyclohexanone
35.03	NCH ₃	dimethylacetamide	66.52	CH ₂	allyl acetate						

References

- (1) Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. *J. Org. Chem.* **1997**, *62*, 7512.
- (2) Except for the compounds in solutions 8–10, as well as the gas samples, hexamethylbenzene, and the corrected values (*vide supra*), all data for the solvents CDCl₃, C₆D₆, (CD₃)₂CO, (CD₃)₂SO, CD₃CN, CD₃OD, and D₂O were previously reported in ref 1.
- (3) A signal for HDO is also observed in (CD₃)₂SO (3.30 ppm) and (CD₃)₂CO (2.81 ppm), often seen as a 1:1:1 triplet ($^2J_{\text{H,D}} = 1$ Hz).
- (4) Splitting pattern observed as a triplet of a non-first-order ABX pattern.
- (5) Not all OH signals were observable.
- (6) In some solvents, the coupling interaction between the CH₂ and the OH protons may be observed ($J = 5$ Hz).
- (7) In CD₃CN, the OH proton was seen as a multiplet at 2.69 ppm, as well as extra coupling to the CH₂ peak.
- (8) Apiezon-brand H grease.
- (9) In some solvents, the coupling interaction between the CH₃ and the OH protons may be observed ($J = 5.5$ Hz).
- (10) Pyrrolidine was observed to react with the solvent (CD₃)₂CO.
- (11) Phosphorus coupling was observed ($^2J_{\text{PC}} = 3$ Hz).
- (12) Internal reference; see Experimental Section in text.