Supporting Information

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

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Corrections and Comments

In the preparation of this manuscript, several errors were discovered in the original paper[1] and are reported herein. While comparing the ^{1}H NMR spectral data obtained in toluene-d_8 to that in C_6D_6, it was discovered that the ^{1}H NMR chemical shifts for acetic acid (C*H*$_3$), acetonitrile (C*H*$_3$) and *tert*-butyl alcohol (O*H*) in C_6D_6 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 C_6D_6, $(CD_3)_2CO$, $(CD_3)_2SO$, CD_3CN, and CD_3OD were reversed and are now corrected. The resonances for 1,2-dimethoxyethane (*C*H$_2$) in $(CD_3)_2CO$, silicone grease (*C*H$_3$) in $CDCl_3$, and 2-propanol (C*H*$_3$) in CD_3OD 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 O*H* resonance for ethanol in C_6D_6 (0.50 ppm), the C*H*$_3$ resonance for silicone grease in $(CD_3)_2SO$ (–0.06 ppm), and replaced the “grease” entry (formerly motor oil[1]) with VWR vacuum pump oil #19, which is now reported in each deuterated solvent.

Table S1. [1]H NMR Data[2]

	proton	mult	THF-d_8	CD_2Cl_2	$CDCl_3$	toluene-d_8	C_6D_6	C_6D_5Cl	$(CD_3)_2CO$	$(CD_3)_2SO$	CD_3CN	TFE-d_3	CD_3OD	D_2O
solvent residual signals			1.72 3.58	5.32	7.26	2.08 6.97 7.01 7.09	7.16	6.96 6.99 7.14	2.05	2.50	1.94	5.02 3.88	3.31	4.79
water	OH	s	2.46	1.52	1.56	0.43	0.40	1.03	2.84[3]	3.33[3]	2.13	3.66	4.87	-
acetic acid	CH_3	s	1.89	2.06	2.10	1.57	1.52	1.76	1.96	1.91	1.96	2.06	1.99	2.08
acetone	CH_3	s	2.05	2.12	2.17	1.57	1.55	1.77	2.09	2.09	2.08	2.19	2.15	2.22
acetonitrile	CH_3	s	1.95	1.97	2.10	0.69	0.58	1.21	2.05	2.07	1.96	1.95	2.03	2.06
allyl acetate	C***H***CH_2	ddt	5.90	5.92	5.93	5.67[4]	5.68[4]	5.77	5.92	5.91	5.93	5.93	5.94	5.99
	CHC***H***$_2$(1)	ddt	5.27	5.31	5.32	5.05	5.06	5.15	5.29	5.29	5.29	5.32	5.30	5.37
	CHC***H***$_2$(2)	ddt	5.15	5.22	5.24	4.94	4.94	5.04	5.18	5.20	5.21	5.25	5.21	5.30
	CH_2	ddd	4.50	4.55	4.57	4.34	4.38	4.44	4.53	4.52	4.53	4.58	4.56	4.62
	CH_3	s	1.98	2.05	2.09	1.63	1.63	1.80	2.02	2.03	2.02	2.07	2.05	2.13
benzaldehyde	HCO	s	9.98	10.01	10.03	9.57	9.64	9.77	10.05	10.02	10.01	9.88	10.00	9.96
	CH(2,6)	m	7.86–7.88	7.87–7.89	7.88–7.91	7.45–7.47	7.49–7.53	7.59–7.61	7.92–7.94	7.91–7.93	7.89–7.91	7.90–7.92	7.90–7.93	7.97–7.99
	CH(3,5)	m	7.51–7.55	7.53–7.57	7.51–7.57	6.95–6.99	6.93–6.99	7.15–7.19	7.59–7.63	7.61–7.67	7.57–7.61	7.56–7.59	7.56–7.60	7.57–7.66
	CH(4)	m	7.60–7.64	7.63–7.67	7.61–7.65	7.03–7.07	7.01–7.07	7.24–7.28	7.69–7.73	7.69–7.75	7.67–7.71	7.68–7.72	7.66–7.70	7.76–7.80
benzene	CH	s	7.31	7.35	7.36	7.12	7.15	7.20	7.36	7.37	7.37	7.36	7.33	-
tert-butyl alcohol	CH_3	s	1.15	1.24	1.28	1.03	1.05	1.12	1.18	1.11	1.16	1.28	1.40	1.24
	OH	s[5]	3.16	-	-	0.58	0.63	1.30	-	4.19	2.18	2.20	-	-
BHA	ArH	s	6.68	6.73	6.76	6.83	6.93	6.83	6.72	6.62	6.73	6.87	6.71	-
	OH	s[5]	5.64	4.76	4.76	4.45	4.53	4.62	5.65	6.52	4.98	-	4.85	-
	$ArOCH_3$	s	3.68	3.73	3.77	3.48	3.48	3.61	3.72	3.66	3.72	3.79	3.72	-
	$ArC(CH_3)_3$	s	1.40	1.42	1.44	1.34	1.41	1.37	1.41	1.36	1.40	1.44	1.41	-
BHT	ArH	s	6.92	6.97	6.98	6.99	7.05	6.97	6.96	6.87	6.97	7.06	6.92	-
	OH	s[5]	5.81	5.00	5.01	4.72	4.79	5.50	-	6.65	5.20	-	-	-
	$ArCH_3$	s	2.21	2.25	2.27	2.23	2.24	2.20	2.22	2.18	2.22	2.24	2.21	-
	$ArC(CH_3)_3$	s	1.40	1.42	1.43	1.36	1.38	1.37	1.41	1.36	1.39	1.43	1.40	-
chloroform	CH	s	7.89	7.32	7.26	6.10	6.15	6.74	8.02	8.32	7.58	7.33	7.90	-
18-crown-6	CH_2	s	3.57	3.59	3.67	3.36	3.39	3.41	3.59	3.51	3.51	3.64	3.64	3.80
cyclohexane	CH_2	s	1.44	1.44	1.43	1.40	1.40	1.37	1.43	1.40	1.44	1.47	1.45	-
cyclohexanone	CH_2(2,6)	t	2.24	2.29	2.33	1.95	1.98	2.08	2.27	2.25	2.27	2.38	2.34	2.40
	CH_2(3,5)	m	1.77–1.82	1.81–1.87	1.84–1.86	1.33–1.39	1.28–1.37	1.48–1.53	1.79–1.83	1.74–1.78	1.79–1.84	1.87–1.92	1.85–1.87	1.85–1.90
	CH_2(4)	m	1.68–1.71	1.69–1.72	1.71–1.73	1.16–1.20	1.08–1.16	1.33–1.37	1.70–1.74	1.64–1.66	1.67–1.72	1.75–1.78	1.74–1.76	1.70–1.75
diallyl carbonate	C***H***CH_2	ddt	5.92	5.95	5.94	5.63	5.65	5.75	5.96	5.93	5.96	5.92	5.94	5.99
	CHC***H***$_2$(1)	ddt	5.31	5.35	5.37	5.09	5.09	5.17	5.35	5.33	5.34	5.35	5.34	5.40
	CHC***H***$_2$(2)	ddt	5.19	5.26	5.27	4.92	4.92	5.03	5.23	5.25	5.25	5.28	5.25	5.32
	CH_2	ddd	4.58	4.61	4.64	4.34	4.38	4.46	4.62	4.61	4.61	4.62	4.61	4.69
1,2-dichloroethane	CH_2	s	3.77	3.76	3.73	2.91	2.90	3.26	3.87	3.90	3.81	3.71	3.78	-
dichloromethane	CH_2	s	5.51	5.33	5.30	4.32	4.27	4.77	5.63	5.76	5.44	5.24	5.49	-
diethyl ether	CH_3	t, 7	1.12	1.15	1.21	1.10	1.11	1.10	1.11	1.09	1.12	1.20	1.18	1.17
	CH_2	q, 7	3.38	3.43	3.48	3.25	3.26	3.31	3.41	3.38	3.42	3.58	3.49	3.56
diglyme	CH_2	m	3.43	3.57	3.65	3.43	3.46	3.49	3.56	3.51	3.53	3.67	3.61	3.67
	CH_2	m	3.53	3.50	3.57	3.31	3.34	3.37	3.47	3.38	3.45	3.62	3.58	3.61
	OCH_3	s	3.28	3.33	3.39	3.12	3.11	3.16	3.28	3.24	3.29	3.41	3.35	3.37
1,2-dimethoxyethane	CH_3	s	3.28	3.34	3.40	3.12	3.12	3.17	3.28	3.24	3.28	3.40	3.35	3.37
	CH_2	s	3.43	3.49	3.55	3.31	3.33	3.37	3.46	3.43	3.45	3.61	3.52	3.60
dimethylacetamide	CH_3CO	s	1.94	2.02	2.09	1.59	1.60	1.74	1.97	1.96	1.97	2.09	2.07	2.08
	NCH_3	s	2.95	2.97	3.02	2.56	2.57	2.65	3.00	2.94	2.96	3.05	3.31	3.06
	NCH_3	s	2.82	2.87	2.94	2.11	2.05	2.42	2.83	2.78	2.83	2.94	2.92	2.90
dimethyl carbonate	CH_3	s	3.69	3.75	3.79	3.31	3.30	3.48	3.72	3.69	3.72	3.77	3.74	3.69
dimethyl malonate	CH_3	s	3.65	3.72	3.75	3.24	3.23	3.41	3.68	3.65	3.68	3.76	3.72	3.78
	CH_2	s	3.35	3.37	3.40	2.92	2.97	3.15	3.42	3.53	3.38	3.41	3.44	3.60
dimethylformamide	CH	s	7.91	7.96	8.02	7.57	7.63	7.73	7.96	7.95	7.92	7.86	7.97	7.92
	CH_3	s	2.88	2.91	2.96	2.37	2.36	2.51	2.94	2.89	2.89	2.98	2.99	3.01
	CH_3	s	2.76	2.82	2.88	1.96	1.86	2.30	2.78	2.73	2.77	2.88	2.86	2.85
dimethyl sulfoxide	CH_3	s	2.45	2.55	2.62	1.64	1.68	2.03	2.52	2.54	2.50	2.63	2.65	2.71
1,4-dioxane	CH_2	s	3.56	3.65	3.71	3.33	3.35	3.45	3.59	3.57	3.60	3.76	3.66	3.75
ethane	CH_3	s	0.85	0.85	0.87	0.81	0.80	0.79	0.83	0.82	0.85	0.85	0.85	0.82
ethanol	CH_3	t, 7	1.10	1.19	1.25	0.97	0.96	1.06	1.12	1.06	1.12	1.22	1.19	1.17
	CH_2	q, 7[6]	3.51	3.66	3.72	3.36	3.34	3.51	3.57	3.44	3.54	3.71	3.60	3.65
	OH	s[5,6]	3.30	1.33	1.32	0.83	0.50	1.39	3.39	4.63	2.47	-	-	-
ethyl acetate	CH_3CO	s	1.94	2.00	2.05	1.69	1.65	1.78	1.97	1.99	1.97	2.03	2.01	2.07
	C***H***$_2CH_3$	q, 7	4.04	4.08	4.12	3.87	3.89	3.96	4.05	4.03	4.06	4.14	4.09	4.14
	CH_2C***H***$_3$	t, 7	1.19	1.23	1.26	0.94	0.92	1.04	1.20	1.17	1.20	1.26	1.24	1.24
ethyl methyl ketone	CH_3CO	s	2.03	2.09	2.14	1.59	1.58	1.78	2.07	2.07	2.06	2.16	2.12	2.19
	C***H***$_2CH_3$	q, 7	2.39	2.43	2.46	1.82	1.81	2.06	2.45	2.43	2.43	2.49	2.50	3.18
	CH_2C***H***$_3$	t, 7	0.96	1.00	1.06	0.84	0.85	0.89	0.96	0.91	0.96	1.05	1.01	1.26
ethylene	CH_2	s	5.36	5.40	5.40	5.25	5.25	5.29	5.38	5.41	5.41	5.40	5.39	5.44
ethylene glycol	CH_2	s[7]	3.48	3.66	3.76	3.36	3.41	3.58	3.28	3.34	3.51	3.72	3.59	3.65
furan	CH(2,5)	dd	7.48	7.46	7.45	7.10	7.13	7.24	7.56	7.67	7.52	7.44	7.49	7.57
	CH(3,4)	dd	6.37	6.41	6.40	6.07	6.08	6.19	6.43	6.47	6.44	6.42	6.40	6.51
H grease[8]	CH_3	m	0.85–0.91	0.84–0.90	0.84–0.87	0.89–0.96	0.90–0.98	0.86–0.92	0.90	0.82–0.88	-	0.88–0.94	0.86–0.93	-
	CH_2	br s	1.29	1.27	1.25	1.33	1.32	1.30	1.29	1.24	-	1.33	1.29	-
hexamethylbenzene	CH_3	s	2.18	2.20	2.24	2.10	2.13	2.10	2.17	2.14	2.19	2.24	2.19	-
hexamethyldisiloxane	CH_3	s	0.07	0.07	0.07	0.10	0.12	0.10	0.07	0.06	0.07	0.08	0.07	0.28

n -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
n -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

Table S2. $^{13}C\{^{1}H\}$ NMR Data[2]

	carbon	THF-d_8	CD_2Cl_2	$CDCl_3$	toluene-d_8	C_6D_6	C_6D_5Cl	$(CD_3)_2CO$	$(CD_3)_2SO$	CD_3CN	TFE-d_3	CD_3OD	D_2O
solvent signals		67.21 25.31	53.84	77.16	137.48 128.87 127.96 125.13 20.43	128.06	134.19 129.26 128.25 125.96	29.84 206.26	39.52	1.32 118.26	61.50 126.28	49.00	-
acetic acid	CO	171.69	175.85	175.99	175.30	175.82	175.67	172.31	171.93	173.21	177.96	175.11	177.21
	CH_3	20.13	20.91	20.81	20.27	20.37	20.40	20.51	20.95	20.73	20.91	20.56	21.03
acetone	CO	204.19	206.78	207.07	204.00	204.43	204.83	205.87	206.31	207.43	32.35	209.67	215.94
	CH_3	30.17	31.00	30.92	30.03	30.14	30.12	30.60	30.56	30.91	214.98	30.67	30.89
acetonitrile	CN	116.79	116.92	116.43	115.76	116.02	115.93	117.60	117.91	118.26	118.95	118.06	119.68
	CH_3	0.45	2.03	1.89	0.03	0.20	0.63	1.12	1.03	1.79	1.00	0.85	1.47
allyl acetate	CO	170.14	170.83	170.81	169.44	169.67	169.59	170.61	169.97	171.32	175.98	172.41	174.78
	$\boldsymbol{C}HCH_2$	133.90	132.94	132.33	132.98	132.90	132.69	133.76	132.71	133.83	133.33	133.71	132.48
	$CH\boldsymbol{C}H_2$	117.58	118.00	118.34	117.49	117.64	117.63	117.81	117.64	118.06	119.39	118.22	119.03
	CH_2	65.31	65.36	65.28	64.87	64.92	64.86	65.28	64.32	65.55	67.61	66.14	66.52
	CH_3	20.45	21.06	21.02	20.21	20.37	20.40	20.68	20.54	21.02	21.10	20.71	21.00
benzaldehyde	HCO	191.95	192.61	192.67	191.09	191.43	191.24	192.95	193.08	193.64	197.63	194.11	191.67
	C(1)	137.78	136.98	136.58	137.12	137.05	136.78	137.66	136.20	137.62	137.84	137.96	136.11
	CH(2,6)	129.98	129.98	129.91	129.61	129.65	129.49	130.23	129.45	130.42	131.78	130.64	130.09
	CH(3,5)	129.56	129.42	129.16	128.68	128.95	128.87	129.90	129.10	130.07	130.82	130.12	129.48
	CH (4)	134.67	134.79	134.64	133.88	133.95	134.02	135.14	134.52	135.40	137.17	135.60	134.70
benzene	CH	128.84	128.68	128.37	128.57	128.62	128.38	129.15	128.30	129.32	129.84	129.34	-
tert -butyl alcohol	$(CH_3)_3\boldsymbol{C}$	67.50	69.11	69.15	68.12	68.19	68.19	68.13	66.88	68.74	72.35	69.40	70.36
	$(\boldsymbol{C}H_3)_3C$	30.57	31.46	31.25	30.49	30.47	31.13	30.72	30.38	30.68	31.07	30.91	30.29
BHA	C(1)	154.07	153.05	152.57	153.50	153.62	153.19	153.97	152.53	154.02	153.74	154.34	-
	C(2,6)	148.62	148.06	147.85	148.06	148.13	147.87	148.48	147.44	148.39	150.52	149.04	-
	CH(3,5)	110.94	110.93	110.69	110.99	111.15	110.84	111.00	109.80	111.35	112.90	111.30	-
	C(4)	140.07	137.77	137.36	137.34	137.50	137.29	140.32	141.16	140.20	140.23	141.36	-
	CH_3O	55.39	55.88	55.70	55.04	55.27	55.08	55.51	54.89	55.94	57.55	55.96	-
	$(\boldsymbol{C}H_3)_3C$	30.65	30.37	30.32	30.30	30.35	30.21	30.64	30.30	30.55	30.80	30.82	-
	$(CH_3)_3\boldsymbol{C}$	35.51	34.91	34.72	34.69	34.72	34.56	35.45	34.76	35.48	36.07	35.83	-
BHT	C(1)	152.48	151.92	151.55	152.06	152.05	151.69	152.51	151.47	152.42	153.46	152.85	-
	C(2,6)	137.93	136.32	135.87	136.12	136.08	135.92	138.19	139.12	138.13	138.59	139.09	-
	CH(3,5)	125.71	125.84	125.55	125.79	125.83	125.58	126.03	124.85	126.38	127.11	126.11	-
	C(4)	128.64	128.73	128.27	128.44	128.52	128.26	129.05	127.97	129.61	130.62	129.49	-
	CH_3Ar	21.21	21.27	21.20	21.42	21.40	21.10	21.31	20.97	21.23	21.34	21.38	-
	$(\boldsymbol{C}H_3)_3C$	31.55	30.54	30.33	31.39	31.34	30.19	31.61	31.25	31.50	31.01	31.15	-
	$(CH_3)_3\boldsymbol{C}$	34.91	34.56	34.25	34.39	34.35	34.11	35.00	34.33	35.05	35.69	35.36	-
carbon dioxide	CO_2	125.69	125.26	124.99	124.86	124.76	126.08	125.81	124.21	125.89	126.92	126.31	-
carbon disulfide	CS_2	193.37	192.95	192.83	192.71	192.69	192.49	193.58	192.63	193.60	196.26	193.82	197.25
carbon tetrachloride	CCl_4	96.89	96.52	96.34	96.57	96.44	96.38	96.65	95.44	96.68	97.74	97.21	96.73
chloroform	CH	79.24	77.99	77.36	77.89	77.79	77.67	79.19	79.16	79.17	78.83	79.44	-
18-crown-6	CH_2	71.34	70.47	70.55	70.86	70.59	70.55	71.25	69.85	71.22	70.80	71.47	70.14
cyclohexane	CH_2	27.58	27.38	26.94	27.31	27.23	26.99	27.51	26.33	27.63	28.34	27.96	-
cyclohexanone	CO	208.79	211.82	212.57	208.60	209.10	209.30	210.36	210.63	211.99	221.30	214.69	221.22
	CH_2(2,6)	42.17	42.31	41.97	41.78	41.83	41.79	42.24	41.32	42.44	43.16	42.61	42.02
	CH_2(3,5)	27.69	27.47	27.00	27.05	27.00	27.02	27.68	26.46	27.80	28.56	28.16	27.50
	CH_2(4)	25.76	25.42	24.97	25.15	25.03	25.07	25.59	24.32	25.62	26.00	25.86	24.77
diallyl carbonate	CO	155.36	155.15	154.88	155.15	155.24	154.87	155.48	154.16	155.66	157.39	156.28	157.78
	$\boldsymbol{C}HCH_2$	133.08	132.24	131.58	132.30	132.18	131.93	133.16	132.18	133.20	132.72	133.25	132.76
	$CH\boldsymbol{C}H_2$	117.70	118.75	118.96	118.04	118.22	118.22	118.53	118.32	118.86	120.15	118.74	118.75
	CH_2	68.58	68.76	68.55	68.20	68.28	68.19	68.78	67.86	69.09	70.69	69.35	68.81
1,2-dichloroethane	CH_2	44.64	44.35	43.50	43.40	43.59	43.60	45.25	45.02	45.54	45.28	45.11	-
dichloromethane	CH_2	54.67	54.24	53.52	53.47	53.46	53.54	54.95	54.84	55.32	54.46	54.78	-
diethyl ether	CH_3	15.49	15.44	15.20	15.47	15.46	15.35	15.78	15.12	15.63	15.33	15.46	14.77
	CH_2	66.14	66.11	65.91	65.94	65.94	65.79	66.12	62.05	66.32	67.55	66.88	66.42
diglyme	CH_3	58.72	58.95	59.01	58.62	58.66	58.42	58.77	57.98	58.90	59.40	59.06	58.67
	CH_2	71.17	70.70	70.51	70.92	70.87	70.56	71.03	69.54	70.99	73.05	71.33	70.05
	CH_2	72.72	72.25	71.90	72.39	72.35	72.07	72.63	71.25	72.63	71.33	72.92	71.63
1,2-dimethoxyethane	CH_3	58.72	59.02	59.08	58.63	58.68	58.31	58.45	58.03	58.89	59.52	59.06	58.67
	CH_2	72.58	72.24	71.84	72.25	72.21	71.81	72.47	71.17	72.47	72.87	72.72	71.49
dimethylacetamide	CH_3	21.15	21.64	21.53	21.05	21.16	21.03	21.51	21.29	21.76	21.40	21.32	21.09
	CO	169.77	171.05	171.07	169.65	169.95	169.79	170.61	169.54	171.31	175.74	173.32	174.57
	NCH_3	34.60	35.23	35.28	34.58	34.67	34.59	34.89	34.42	35.17	36.28	35.50	35.03
	NCH_3	37.56	38.22	38.13	36.98	37.03	37.13	37.92	37.38	38.26	39.06	38.43	38.76
dimethyl carbonate	CO	156.91	156.73	156.45	156.61	156.71	156.36	157.04	155.76	157.26	159.04	157.91	163.96
	CH_3	54.58	55.09	54.89	54.13	54.30	54.23	54.95	54.63	55.39	56.17	55.25	55.81
dimethyl malonate	CO_2	167.14	167.32	167.18	166.49	166.66	166.51	167.58	166.91	168.07	170.88	168.70	170.12
	CH_3	52.07	52.75	52.57	51.76	51.86	51.89	52.47	52.08	52.95	54.00	52.83	53.65
	CH_2	41.15	41.48	41.11	40.88	41.04	40.93	41.43	40.72	41.77	42.13	41.60	42.13
dimethylformamide	CH	161.96	162.57	162.62	161.93	162.13	162.01	162.79	162.29	163.31	166.01	164.73	165.53
	CH_3	35.65	36.56	36.50	35.22	35.25	35.45	36.15	35.73	36.57	37.76	36.89	37.54
	CH_3	30.70	31.39	31.45	30.64	30.72	30.71	31.03	30.73	31.32	30.96	31.61	32.03
dimethyl sulfoxide	CH_3	41.21	41.33	40.76	40.41	40.03	40.27	41.23	40.45	41.31	40.06	40.45	39.39
1,4-dioxane	CH_2	67.65	67.47	67.14	67.17	67.16	66.95	67.60	66.36	67.72	68.52	68.11	67.19
ethane	CH_3	6.79	6.91	6.89	6.94	6.96	6.91	6.88	6.61	6.99	7.01	6.98	-
ethanol	CH_3	18.90	18.69	18.41	18.78	18.72	18.55	18.89	18.51	18.80	18.11	18.40	17.47
	CH_2	57.60	58.57	58.28	57.81	57.86	57.63	57.72	56.07	57.96	59.68	58.26	58.05

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
	CH_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_2***C***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
n -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
n -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	-
	CH(4)	125.84	125.62	125.33	125.66	125.68	125.43	126.12	125.29	126.28	126.82	126.29	-
triethylamine	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 (^{1}H 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	C***H***$_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	CHC***H***$_2$(2)	allyl acetate
0.89	t, 7	CH_3	*n*-hexane	2.46	q, 7	CH_2	triethylamine	5.19	ddt	CHC***H***$_2$(2)	diallyl carbonate
0.89	t, 7	CH_3	*n*-pentane	2.58	d, 9.5	CH_3	HMPA	5.27	ddt	CHC***H***$_2$(1)	allyl acetate
0.90	t, 7.3	CH_3	propane	2.75	m	CH_2(2,5)	pyrrolidine	5.31	ddt	CHC***H***$_2$(1)	diallyl carbonate
0.96	t, 7	CH_2C***H***$_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[9]	OH	methanol	5.81	s	OH	BHT
1.15	s	CH_3	*tert*-butyl alcohol	3.16	s	OH	*tert*-butyl alcohol	5.90	ddt	C***H***CH_2	allyl acetate
1.19	t, 7	CH_2C***H***$_3$	ethyl acetate	3.27	s[9]	CH_3	methanol	5.92	ddt	C***H***CH_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	*n*-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[6]	OH	ethanol	6.66	m	CH(2,5)	pyrrole
1.31	m	CH_2	*n*-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[6]	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_3CO	dimethylacetamide	3.68	s	$ArOCH_3$	BHA	7.86–7.88	m	CH(2,6)	benzaldehyde
1.94	s	CH_3CO	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_3CO	ethyl methyl ketone	4.04	q, 7	C***H***$_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}C{^{1}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_3	silicone grease	30.57	(CH$_3$)$_3$C	*tert*-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_2CH_3	ethyl methyl ketone	30.70	CH_3	dimethylformamide	67.50	(CH$_3$)$_3$$C$	*tert*-butyl alcohol	133.90	CHCH$_2$	allyl acetate
12.51	CH_3	triethylamine	31.55	(CH$_3$)$_3$C	BHT	67.65	CH_2	1,4-dioxane	134.02	CH	propylene
14.18	CH_3	*n*-pentane	32.34	CH_2(3,4)	*n*-hexane	68.03	CH_2(2,5)	tetrahydrofuran	134.67	CH (4)	benzaldehyde
14.22	CH_3	*n*-hexane	34.60	NCH_3	dimethylacetamide	68.58	CH_2	diallyl carbonate	135.72	CH(2)	imidazole
14.37	CH_3	ethyl acetate	34.87	CH_2(3)	*n*-pentane	71.17	CH_2	diglyme	135.99	CH(4)	pyridine
15.49	CH_3	diethyl ether	34.91	(CH$_3$)$_3$$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_3	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$_3$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_3Ar	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)	*n*-pentane	49.64	CH_3	methanol	118.03	CH(2,5)	pyrrole	167.14	CO_2	dimethyl malonate
23.33	CH_2(2,5)	*n*-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_3O	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$_3$CO	ethyl methyl ketone	62.49	CH_3	nitromethane	128.84	CH	benzene	208.79	CO	cyclohexanone

Table S5. CD_2Cl_2 (^{1}H 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_3CO	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	CHC***H***$_2$(2)	allyl acetate
0.89	t, 7	CH_3	n-hexane	2.43	q, 7	C***H***$_2$CH$_3$	ethyl methyl ketone	5.26	ddt	CHC***H***$_2$(2)	diallyl carbonate
0.89	t, 7	CH_3	n-pentane	2.48	q, 7	CH_2	triethylamine	5.31	ddt	CHC***H***$_2$(1)	allyl acetate
0.90	t, 7.3	CH_3	propane	2.55	s	CH_3	dimethyl sulfoxide	5.32	t	$CDHCl_2$	CD_2Cl_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	$CH_2C\boldsymbol{H}_3$	ethyl methyl ketone	2.82	s	CH_3	dimethylformamide	5.35	ddt	CHC***H***$_2$(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	C***H***CH_2	allyl acetate
1.19	t, 7	CH_3	ethanol	2.97	s	NCH_3	dimethylacetamide	5.95	ddt	C***H***CH_2	diallyl carbonate
1.23	t, 7	$CH_2C\boldsymbol{H}_3$	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[6]	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[6]	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_3CO	ethyl acetate	4.08	q, 7	C***H***$_2$CH$_3$	ethyl acetate	8.59	m	CH(2,6)	pyridine
2.02	s	CH_3CO	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. CD_2Cl_2 (^{13}C{^{1}H} 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	(***C***H$_3$)$_3$C	BHA	64.67	CH	2-propanol	129.98	CH(2,6)	benzaldehyde
1.96	CH_3	hexamethyldisiloxane	30.54	(***C***H$_3$)$_3$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	$CH_2\boldsymbol{C}H_3$	ethyl methyl ketone	31.46	(***C***H$_3$)$_3$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[i]	77.99	CH	chloroform	138.36	C(1)	toluene
16.93	CH_3	hexamethylbenzene	37.01	CH_2CH_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_3CO	ethyl acetate	44.35	CH_2	1,2-dichloroethane	116.92	CN	acetonitrile	155.15	CO	diallyl carbonate
21.27	CH_3Ar	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	$CH\boldsymbol{C}H_2$	allyl acetate	162.57	CH	dimethylformamide
21.64	CH_3	dimethylacetamide	50.45	CH_3	methanol	118.75	$CH\boldsymbol{C}H_2$	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_2Cl_2	CD_2Cl_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_3O	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_3CO	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. $CDCl_3$ (^{1}H 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_3CO	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	CHC***H***$_2$(2)	allyl acetate
0.88	t, 7	CH_3	*n*-hexane	2.46	q, 7	C***H***$_2$CH$_3$	ethyl methyl ketone	5.27	ddt	CHC***H***$_2$(2)	diallyl carbonate
0.88	t, 7	CH_3	*n*-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	CHC***H***$_2$(1)	allyl acetate
1.03	t, 7	CH_3	triethylamine	2.65	d, 9.5	CH_3	HMPA	5.37	ddt	CHC***H***$_2$(1)	diallyl carbonate
1.06	t, 7	CH$_2$C***H***$_3$	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	C***H***CH$_2$	allyl acetate
1.22	d, 6	CH_3	2-propanol	2.96	s	CH_3	dimethylformamide	5.94	ddt	C***H***CH$_2$	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$_2$C***H***$_3$	ethyl acetate	3.40	s	CH_3	1,2-dimethoxyethane	6.76	s	ArH	BHA
1.26	m	CH_2	*n*-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	*n*-pentane	3.49	s[9]	CH_3	methanol	7.10	s	CH(4,5)	imidazole
1.28	s	CH_3	*tert*-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_3CO	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	C***H***$_2$CH$_3$	ethyl acetate	8.40	br t	NH	pyrrole
2.09	s	CH_3CO	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. $CDCl_3$ (^{13}C{^{1}H} 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	(***C***H$_3$)$_3$C	BHA	65.28	CH_2	allyl acetate	129.91	CH(2,6)	benzaldehyde
1.89	CH_3	acetonitrile	30.33	(***C***H$_3$)$_3$C	BHT	65.91	CH_2	diethyl ether	131.58	***C***HCH$_2$	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	(***C***H$_3$)$_3$C	*tert*-butyl alcohol	67.97	CH_2(2,5)	tetrahydrofuran	132.33	***C***HCH$_2$	allyl acetate
7.86	CH_2CH_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)	*n*-hexane	69.15	(CH$_3$)$_3$***C***	*tert*-butyl alcohol	134.64	CH (4)	benzaldehyde
14.08	CH_3	*n*-pentane	34.16	CH_2(3)	*n*-pentane	70.51	CH_2	diglyme	135.38	CH(2)	imidazole
14.14	CH_3	*n*-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[l]	77.36	CH	chloroform	137.89	C(1)	toluene
16.98	CH_3	hexamethylbenzene	36.89	***C***H$_2$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	***C***H$_3$CO	ethyl acetate	43.50	CH_2	1,2-dichloroethane	116.43	CN	acetonitrile	154.88	CO	diallyl carbonate
21.20	CH_3Ar	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	CH***C***H$_2$	allyl acetate	162.62	CH	dimethylformamide
21.53	CH_3	dimethylacetamide	50.41	CH_3	methanol	118.96	CH***C***H$_2$	diallyl carbonate	167.18	CO_2	dimethyl malonate
22.38	CH_2(2,4)	*n*-pentane	52.57	CH_3	dimethyl malonate	122.00	CH(4,5)	imidazole	170.81	CO	allyl acetate
22.70	CH_2(2,5)	*n*-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_3O	BHA	124.99	CO_2	carbon dioxide	175.99	CO	acetic acid
25.56	CH_2(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	***C***H$_3$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 (^{1}H 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[5]	BHA
0.17	s	CH_4	methane	1.69	s	CH_3CO	ethyl acetate	4.50	s	H_2	hydrogen
0.26	s	CH_3	silicone grease	1.82	q, 7	C***H***$_2$CH$_3$	ethyl methyl ketone	4.72	s	OH[5]	BHT
0.43	s	OH	water	1.95	t	CH_2(2,6)	cyclohexanone	4.92	ddt	CHC***H***$_2$(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	CHC***H***$_2$(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[6]	OH	ethanol	2.11	s	NCH_3	dimethylacetamide	5.05	ddt	CHC***H***$_2$(1)	allyl acetate
0.84	t, 7	CH_2C***H***$_3$	ethyl methyl ketone	2.11	s	CH_3	toluene	5.09	ddt	CHC***H***$_2$(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	C***H***CH_2	diallyl carbonate
0.88–0.96	m	CH_3	pump oil	2.39	q, 7	CH_2	triethylamine	5.67[4]	t(nfo ABX)	C***H***CH_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[8]	2.54	m	CH_2(2,5)	pyrrolidine	6.07	dd	CH(3,4)	furan
0.94	t, 7	CH_2C***H***$_3$	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[9]	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[8]	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[6]	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	C***H***$_2$CH$_3$	ethyl acetate	7.71	br t	NH	pyrrole
1.59	s	CH_3CO	dimethylacetamide	4.32	s	CH_2	dichloromethane	8.47	m	CH(2,6)	pyridine
1.59	s	CH_3CO	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}C{^{1}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[8]	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	$(CH_3)_3C$	*tert*-butyl alcohol	132.98	CHCH$_2$	allyl acetate
7.89	CH_2CH_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	$(CH_3)_3C$	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	$(CH_3)_3C$	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[11]	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$_3$CO	ethyl acetate	46.82	CH_2	triethylamine	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_3Ar	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_3O	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. C_6D_6 (^{1}H 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_3CO	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[5]	BHA
0.40	s	OH	water	1.81	q, 7	CH_2CH_3	ethyl methyl ketone	4.79	s	OH[5]	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_2CH_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[4]	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_2CH_3	ethyl acetate	2.57	s	NCH_3	dimethylacetamide	6.08	dd	CH(3,4)	furan
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_6D_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	s	$ArOCH_3$	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_2CH_3	ethyl acetate	8.53	m	CH(2,6)	pyridine
1.58	s	CH_3CO	ethyl methyl ketone	4.27	s	CH_2	dichloromethane	9.64	s	HCO	benzaldehyde
1.60	s	CH_3CO	dimethylacetamide	4.38	ddd	CH_2	allyl acetate				

Table S12. C_6D_6 ($^{13}C\{^1H\}$ 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	$(CH_3)_3C$	BHA	65.94	CH_2	diethyl ether	131.79	C	hexamethylbenzene
2.05	CH_3	hexamethyldisiloxane	30.47	$(CH_3)_3C$	*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_2CH_3	ethyl methyl ketone	31.34	$(CH_3)_3C$	BHT	68.19	$(CH_3)_3C$	*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	$(CH_3)_3C$	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	$(CH_3)_3C$	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_2CH_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_3CO	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_3Ar	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_3O	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_6D_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_3CO	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. C_6D_5Cl (^{1}H 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_3CO	ethyl methyl ketone	4.62	s	OH[5]	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	C***H***$_2$$CH_3$	ethyl methyl ketone	4.98	dm, 17	CH_2(2)	propylene
0.84	t, 7	CH_3	*n*-pentane	2.08	t	CH_2(2,6)	cyclohexanone	5.03	ddt	CHC***H***$_2$(2)	diallyl carbonate
0.84	t, 7.3	CH_3	propane	2.10	s	CH_3	hexamethylbenzene	5.04	ddt	CHC***H***$_2$(2)	allyl acetate
0.85	t, 7	CH_3	*n*-hexane	2.16	s	CH_3	toluene	5.15	ddt	CHC***H***$_2$(1)	allyl acetate
0.86–0.92	m	CH_3	H grease[8]	2.20	s	$ArCH_3$	BHT	5.17	ddt	CHC***H***$_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_2C***H***$_3$	ethyl methyl ketone	2.39	q, 7	CH_2	triethylamine	5.50	s	OH[5]	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	C***H***CH_2	diallyl carbonate
1.04	t, 7	CH_2C***H***$_3$	ethyl acetate	2.51	s	CH_3	dimethylformamide	5.77	ddt	C***H***CH_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	*tert*-butyl alcohol	3.16	s	OCH_3	diglyme	6.74	s	CH	chloroform
1.19	m	CH_2	*n*-hexane	3.17	s	CH_3	1,2-dimethoxyethane	6.83	s	ArH	BHA
1.21	s	CH_3	acetonitrile	3.25	s[9]	CH_3	methanol	6.90	m	CH(3,5)	pyridine
1.23	m	CH_2	*n*-pentane	3.26	s	CH_2	1,2-dichloroethane	6.96	br. s	CH(4)	C_6D_5Cl 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	*tert*-butyl alcohol	3.37	m	CH_2	diglyme	6.99	br. s	CH(3,5)	C_6D_5Cl residual
1.30	br s	CH_2	H grease[8]	3.37	s	CH_2	1,2-dimethoxyethane	7.01	s	CH(4,5)	imidazole
1.30	s[9]	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_6D_5Cl 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[6]	CH_2	ethanol	7.24	dd	CH(2,5)	furan
1.39	s[6]	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_3CO	dimethylacetamide	3.96	q, 7	C***H***$_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_3CO	ethyl acetate	4.49	s	H_2	hydrogen				

Table S14. C_6D_5Cl ($^{13}C\{^1H\}$ 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_6D_5Cl signal
0.63	CH_3	acetonitrile	30.19	(***C***H_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	(***C***H_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***	*tert*-butyl alcohol	131.93	***C***HCH_2	diallyl carbonate
6.91	CH_3	ethane	31.13	(***C***H_3)$_3$C	*tert*-butyl alcohol	68.19	CH_2	diallyl carbonate	132.69	***C***HCH_2	allyl acetate
7.79	CH_2***C***H_3	ethyl methyl ketone	31.77	CH_2(3,4)	*n*-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)	*n*-pentane	71.81	CH_2	1,2-dimethoxyethane	134.19	CCl	C_6D_5Cl signal
14.10	CH_3	*n*-pentane	34.56	$(CH_3)_3$***C***	BHA	72.07	CH_2	diglyme	135.32	CH(4)	pyridine
14.18	CH_3	*n*-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	***C***H_2CH_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[11]	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	CH***C***H_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	***C***H_3CO	ethyl acetate	46.36	CH_2	triethylamine	118.22	CH***C***H_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_3Ar	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)	*n*-pentane	53.54	CH_2	dichloromethane	125.43	CH(4)	toluene	166.51	CO_2	dimethyl malonate
22.86	CH_2(2,5)	*n*-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_3O	BHA	125.96 (t)	CD(4)	C_6D_5Cl 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_6D_5Cl 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	***C***H_3CO	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[8]	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. $(CD_3)_2CO$ (^{1}H 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	C$\boldsymbol{H}_2$$CH_3$	ethyl methyl ketone	5.18	ddt	CHC$\boldsymbol{H}_2$(2)	allyl acetate
0.88	t, 7	CH_3	*n*-hexane	2.45	q, 7	CH_2	triethylamine	5.23	ddt	CHC$\boldsymbol{H}_2$(2)	diallyl carbonate
0.88	t, 7	CH_3	*n*-pentane	2.52	s	CH_3	dimethyl sulfoxide	5.29	ddt	CHC$\boldsymbol{H}_2$(1)	allyl acetate
0.88	t, 7.3	CH_3	propane	2.59	d, 9.5	CH_3	HMPA	5.35	ddt	CHC$\boldsymbol{H}_2$(1)	diallyl carbonate
0.90	m	CH_3	H grease[8]	2.78	s	CH_3	dimethylformamide	5.38	s	CH_2	ethylene
0.96	t, 7	CH_2C$\boldsymbol{H}_3$	ethyl methyl ketone	2.83	s	NCH_3	dimethylacetamide	5.63	s	CH_2	dichloromethane
0.96	t, 7	CH_3	triethylamine	2.84[3]	s	OH	water	5.65	s	OH[5]	BHA
1.10	d, 6	CH_3	2-propanol	2.94	s	CH_3	dimethylformamide	5.81	m	CH	propylene
1.11	t, 7	CH_3	diethyl ether	3.00	s	NCH_3	dimethylacetamide	5.92	ddt	C$\boldsymbol{H}$$CH_2$	allyl acetate
1.12	t, 7	CH_3	ethanol	3.12	s[9]	OH	methanol	5.96	ddt	C$\boldsymbol{H}$$CH_2$	diallyl carbonate
1.18	s	CH_3	*tert*-butyl alcohol	3.28	s	OCH_3	diglyme	6.07	m	CH(3,4)	pyrrole
1.20	t, 7	CH_2C$\boldsymbol{H}_3$	ethyl acetate	3.28	s	CH_3	1,2-dimethoxyethane	6.43	dd	CH(3,4)	furan
1.27	m	CH_2	*n*-pentane	3.28	s	CH_2	ethylene glycol	6.72	s	ArH	BHA
1.28	m	CH_2	*n*-hexane	3.31	s[9]	CH_3	methanol	6.77	m	CH(2,5)	pyrrole
1.29	br s	CH_2	H grease[8]	3.39	s[6]	OH	ethanol	6.96	s	ArH	BHT
1.29	br s	CH_2	pump oil	3.41	q, 7	CH_2	diethyl ether	7.04	s	CH(4,5)	imidazole
1.31	sept, 7.3	CH_2	propane	3.42	s	CH_2	dimethyl malonate	7.10–7.20	m	CH(2,4,6)	toluene
1.41	s	$ArC(CH_3)_3$	BHA	3.46	s	CH_2	1,2-dimethoxyethane	7.10–7.20	m	CH(3,5)	toluene
1.41	s	$ArC(CH_3)_3$	BHT	3.47	m	CH_2	diglyme	7.35	m	CH(3,5)	pyridine
1.43	s	CH_2	cyclohexane	3.56	m	CH_2	diglyme	7.36	s	CH	benzene
1.68	dt, 6.4, 1.5	CH_3	propylene	3.57	q, 7[6]	CH_2	ethanol	7.56	dd	CH(2,5)	furan
1.70–1.74	m	CH_2(4)	cyclohexanone	3.59	s	CH_2	18-crown-6	7.59–7.63	m	CH(3,5)	benzaldehyde
1.79	m	CH_2(3,4)	tetrahydrofuran	3.59	s	CH_2	1,4-dioxane	7.62	s	CH(2)	imidazole
1.79–1.83	m	CH_2(3,5)	cyclohexanone	3.63	m	CH_2(2,5)	tetrahydrofuran	7.69–7.73	m	CH(4)	benzaldehyde
1.96	s	CH_3	acetic acid	3.68	s	CH_3	dimethyl malonate	7.76	m	CH(4)	pyridine
1.97	s	CH_3CO	dimethylacetamide	3.72	s	$ArOCH_3$	BHA	7.92–7.94	m	CH(2,6)	benzaldehyde
1.97	s	CH_3CO	ethyl acetate	3.72	s	CH_3	dimethyl carbonate	7.96	s	CH	dimethylformamide
2.02	s	CH_3	allyl acetate	3.87	s	CH_2	1,2-dichloroethane	8.02	s	CH	chloroform
2.05	s	CH_3	acetonitrile	3.90	sept, 6	CH	2-propanol	8.58	m	CH(2,6)	pyridine
2.05	p	CHD_2	$(CD_3)_2CO$ residual	4.05	q, 7	C$\boldsymbol{H}_2$$CH_3$	ethyl acetate	10.02	br t	NH	pyrrole
2.07	s	CH_3CO	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. $(CD_3)_2CO$ (^{13}C{^{1}H} 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	($\boldsymbol{C}H_3)_3$C	BHA	66.12	CH_2	diethyl ether	132.22	C	hexamethylbenzene
1.40	CH_3	silicone grease	30.72	($\boldsymbol{C}H_3)_3$C	*tert*-butyl alcohol	67.60	CH_2	1,4-dioxane	133.16	$\boldsymbol{C}HCH_2$	diallyl carbonate
2.01	CH_3	hexamethyldisiloxane	31.03	CH_3	dimethylformamide	68.07	CH_2(2,5)	tetrahydrofuran	133.76	$\boldsymbol{C}HCH_2$	allyl acetate
6.88	CH_3	ethane	31.61	($\boldsymbol{C}H_3)_3$C	BHT	68.13	$(CH_3)_3\boldsymbol{C}$	*tert*-butyl alcohol	134.34	CH	propylene
8.03	$CH_2\boldsymbol{C}H_3$	ethyl methyl ketone	32.30	CH_2(3,4)	*n*-hexane	68.78	CH_2	diallyl carbonate	135.14	CH (4)	benzaldehyde
12.49	CH_3	triethylamine	34.83	CH_2(3)	*n*-pentane	71.03	CH_2	diglyme	135.89	CH(2)	imidazole
14.29	CH_3	*n*-pentane	34.89	NCH_3	dimethylacetamide	71.25	CH_2	18-crown-6	136.56	CH(4)	pyridine
14.34	CH_3	*n*-hexane	35.00	$(CH_3)_3\boldsymbol{C}$	BHT	72.47	CH_2	1,2-dimethoxyethane	137.66	C(1)	benzaldehyde
14.50	CH_3	ethyl acetate	35.45	$(CH_3)_3\boldsymbol{C}$	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	$\boldsymbol{C}H_2CH_3$	ethyl methyl ketone	96.65	CCl_4	carbon tetrachloride	140.32	C(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	$CH\boldsymbol{C}H_2$	allyl acetate	155.48	CO	diallyl carbonate
20.83	$\boldsymbol{C}H_3CO$	ethyl acetate	47.07	CH_2	triethylamine	117.98	CH(2,5)	pyrrole	157.04	CO	dimethyl carbonate
21.31	CH_3Ar	BHT	49.77	CH_3	methanol	118.53	$CH\boldsymbol{C}H_2$	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)	*n*-pentane	54.95	CH_3	dimethyl carbonate	124.57	CH(3,5)	pyridine	170.61	CO	dimethylacetamide
23.28	CH_2(2,5)	*n*-hexane	55.51	CH_3O	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	$(CD_3)_2CO$ signal
29.30	$\boldsymbol{C}H_3CO$	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	$(CD_3)_2CO$ 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. $(CD_3)_2SO$ (^{1}H 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[6]	OH	ethanol
0.74	m	CH_3	pump oil	2.43	q, 7	CH_2CH_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	$(CD_3)_2SO$ residual	5.20	ddt	$CHCH_2(2)$	allyl acetate
0.86	t, 7	CH_3	*n*-hexane	2.53	d, 9.5	CH_3	HMPA	5.25	ddt	$CHCH_2(2)$	diallyl carbonate
0.86	t, 7	CH_3	*n*-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_2CH_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	*tert*-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_2CH_3	ethyl acetate	3.33[3]	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	*n*-hexane	3.38	q, 7	CH_2	diethyl ether	6.65	s	OH[5]	BHT
1.27	m	CH_2	*n*-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[6]	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_3CO	dimethylacetamide	3.78	sept, 6	CH	2-propanol	7.79	m	CH(4)	pyridine
1.99	s	CH_3CO	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_2CH_3	ethyl acetate	8.58	m	CH(2,6)	pyridine
2.07	s	CH_3CO	ethyl methyl ketone	4.19	s	OH	*tert*-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. $(CD_3)_2SO$ ($^{13}C\{^1H\}$ 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	$(\mathbf{C}H_3)_3C$	*tert*-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	$CH_2(3,4)$	*n*-hexane	66.36	CH_2	1,4-dioxane	132.18	$\mathbf{C}HCH_2$	diallyl carbonate
7.61	$CH_2\mathbf{C}H_3$	ethyl methyl ketone	31.25	$(\mathbf{C}H_3)_3C$	BHT	66.88	$(CH_3)_3\mathbf{C}$	*tert*-butyl alcohol	132.71	$\mathbf{C}HCH_2$	allyl acetate
11.74	CH_3	triethylamine	33.48	$CH_2(3)$	*n*-pentane	67.03	$CH_2(2,5)$	tetrahydrofuran	133.55	CH	propylene
13.28	CH_3	*n*-pentane	34.33	$(CH_3)_3\mathbf{C}$	BHT	67.86	CH_2	diallyl carbonate	134.52	CH (4)	benzaldehyde
13.88	CH_3	*n*-hexane	34.42	NCH_3	dimethylacetamide	69.54	CH_2	diglyme	135.15	CH(2)	imidazole
14.40	CH_3	ethyl acetate	34.76	$(CH_3)_3\mathbf{C}$	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	$\mathbf{C}H_2CH_3$	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	$(CD_3)_2SO$ 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	$\mathbf{C}H_3CO$	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_3Ar	BHT	45.74	CH_2	triethylamine	117.64	$CH\mathbf{C}H_2$	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	$CH\mathbf{C}H_2$	diallyl carbonate	162.29	CH	dimethylformamide
21.70	$CH_2(2,4)$	*n*-pentane	52.08	CH_3	dimethyl malonate	121.55	CH(4,5)	imidazole	166.91	CO_2	dimethyl malonate
22.05	$CH_2(2,5)$	*n*-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_3O	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	$\mathbf{C}H_3CO$	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	$(\mathbf{C}H_3)_3C$	BHA									

Table S19. CD_3CN (^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	*tert*-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	*n*-hexane	2.43	q, 7	CH_2CH_3	ethyl methyl ketone	5.20	s	OH[5]	BHT
0.89	t, 7	CH_3	*n*-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[6]	OH	ethanol	5.25	ddt	$CHCH_2(2)$	diallyl carbonate
0.96	t, 7	CH_2CH_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_2	dichloromethane
1.12	t, 7	CH_3	ethanol	2.77	s	CH_3	dimethylformamide	5.85	m	CH	propylene
1.16	s	CH_3	*tert*-butyl alcohol	2.83	s	NCH_3	dimethylacetamide	5.93	ddt	$CHCH_2$	allyl acetate
1.20	t, 7	CH_2CH_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	*n*-hexane	3.28	s	CH_3	1,2-dimethoxyethane	6.44	dd	CH(3,4)	furan
1.29	m	CH_2	*n*-pentane	3.28	s[9]	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[6]	CH_2	ethanol	7.57	s	CH(2)	imidazole
1.94	p	CHD_2	CD_3CN 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_3CO	dimethylacetamide	3.72	s	$ArOCH_3$	BHA	7.73	m	CH(4)	pyridine
1.97	s	CH_3CO	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_3CO	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_2CH_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[9]	OH	methanol	4.53	ddd	CH_2	allyl acetate				

Table S20. CD_3CN ($^{13}C\{^1H\}$ 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	$(CH_3)_3C$	*tert*-butyl alcohol	65.55	CH_2	allyl acetate	130.07	CH(3,5)	benzaldehyde
1.32 (sept)	CD_3	CD_3CN 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	$(CH_3)_3C$	BHT	68.74	$(CH_3)_3C$	*tert*-butyl alcohol	133.83	$CHCH_2$	allyl acetate
8.14	CH_2CH_3	ethyl methyl ketone	32.36	$CH_2(3,4)$	*n*-hexane	69.09	CH_2	diallyl carbonate	134.78	CH	propylene
12.38	CH_3	triethylamine	34.89	$CH_2(3)$	*n*-pentane	70.99	CH_2	diglyme	135.40	CH (4)	benzaldehyde
14.37	CH_3	*n*-pentane	35.05	$(CH_3)_3C$	BHT	71.22	CH_2	18-crown-6	136.33	CH(2)	imidazole
14.43	CH_3	*n*-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	$(CH_3)_3C$	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_2CH_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_3CN signal	154.02	C(1)	BHA
21.16	CH_3CO	ethyl acetate	47.10	CH_2	triethylamine	118.26	CN	acetonitrile	155.66	CO	diallyl carbonate
21.23	CH_3Ar	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	$CH_2(2,4)$	*n*-pentane	55.32	CH_2	dichloromethane	123.69	CH_2	ethylene	171.31	CO	dimethylacetamide
23.40	$CH_2(2,5)$	*n*-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_3O	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_3CO	ethyl methyl ketone	64.22	CH_2	ethylene glycol	129.94	CH(2,6)	toluene	211.99	CO	cyclohexanone
30.55	$(CH_3)_3C$	BHA	64.30	CH	2-propanol						

Table S21. TFE-d_3 (^{1}H 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	*tert*-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[g]	2.38	t	CH_2(2,6)	cyclohexanone	5.02	s	OH	TFE-d_3 residual
0.90	t, 7	CH_3	*n*-pentane	2.49	q, 7	C***H***$_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	*n*-hexane	2.63	d, 9.5	CH_3	HMPA	5.25	ddt	CHC***H***$_2$(2)	allyl acetate
0.99	m	CH_3	pump oil	2.88	s	CH_3	dimethylformamide	5.28	ddt	CHC***H***$_2$(2)	diallyl carbonate
1.05	t, 7	CH_2C***H***$_3$	ethyl methyl ketone	2.94	s	NCH_3	dimethylacetamide	5.32	ddt	CHC***H***$_2$(1)	allyl acetate
1.20	t, 7	CH_3	diethyl ether	2.98	s	CH_3	dimethylformamide	5.35	ddt	CHC***H***$_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_2C***H***$_3$	ethyl acetate	3.12	q, 7	CH_2	triethylamine	5.92	ddt	C***H***CH_2	diallyl carbonate
1.28	s	CH_3	*tert*-butyl alcohol	3.40	s	CH_3	1,2-dimethoxyethane	5.93	ddt	C***H***CH_2	allyl acetate
1.31	m	CH_2	*n*-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)	furan
1.33	br s	CH_2	H grease[g]	3.44	s	CH_3	methanol	6.84	m	CH(2,5)	pyrrole
1.33	m	CH_2	*n*-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	m	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)	furan
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_3CO	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_3CO	dimethylacetamide	4.05	sept, 6	CH	2-propanol	8.45	m	CH(2,6)	pyridine
2.16	s	CH_3CO	ethyl methyl ketone	4.14	q, 7	C***H***$_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}C{^{1}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$_3$)$_3$C	BHT	67.55	CH_2	diethyl ether	131.78	CH(2,6)	benzaldehyde
2.09	CH_3	hexamethyldisiloxane	31.07	(CH$_3$)$_3$C	*tert*-butyl alcohol	67.61	CH_2	allyl acetate	132.72	***C***HCH_2	diallyl carbonate
2.87	CH_3	silicone grease	31.85	CH_2	pump oil	68.52	CH_2	1,4-dioxane	133.33	***C***HCH_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***C***H_3	ethyl methyl ketone	33.17	CH_2(3,4)	*n*-hexane	70.69	CH_2	diallyl carbonate	136.00	CH	propylene
9.51	CH_3	triethylamine	35.69	(CH_3)$_3$***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)	*n*-pentane	71.33	CH_2	diglyme	137.17	CH (4)	benzaldehyde
14.54	CH_3	*n*-pentane	36.07	(CH_3)$_3$***C***	BHA	72.35	(CH_3)$_3$***C***	*tert*-butyl alcohol	137.84	C(1)	benzaldehyde
14.63	CH_3	*n*-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[i]	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	***C***H$_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)	furan
18.11	CH_3	ethanol	40.06	CH_3	dimethyl sulfoxide	111.06	CH(3,4)	furan	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	***C***H_3CO	ethyl acetate	47.43	CH_2(2,5)	pyrrolidine	119.39	CH***C***H_2	allyl acetate	157.39	CO	diallyl carbonate
21.34	CH_3Ar	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	CH***C***H_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)	*n*-pentane	54.46	CH_2	dichloromethane	124.08	CH_2	ethylene	175.55	CO	ethyl acetate
24.06	CH_2(2,5)	*n*-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_3O	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	***C***H_3CO	ethyl methyl ketone	63.17	CH_3	nitromethane	130.58	CH(2,6)	toluene	221.30	CO	cyclohexanone
30.80	(CH$_3$)$_3$C	BHA	64.87	CH_2	ethylene glycol	130.62	C(4)	BHT			

Table S23. CD_3OD (^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	C***H***$_2$CH$_3$	ethyl methyl ketone	4.91	dm, 10	CH_2(1)	propylene
0.86–0.93	m	CH_3	H grease[g]	2.58	q, 7	CH_2	triethylamine	5.01	dm, 17	CH_2(2)	propylene
0.90	t, 7	CH_3	*n*-hexane	2.64	d, 9.5	CH_3	HMPA	5.21	ddt	CHC***H***$_2$(2)	allyl acetate
0.90	t, 7	CH_3	*n*-pentane	2.65	s	CH_3	dimethyl sulfoxide	5.25	ddt	CHC***H***$_2$(2)	diallyl carbonate
0.91	t, 7.3	CH_3	propane	2.80	m	CH_2(2,5)	pyrrolidine	5.30	ddt	CHC***H***$_2$(1)	allyl acetate
1.01	t, 7	CH_2CH_3	ethyl methyl ketone	2.86	s	CH_3	dimethylformamide	5.34	ddt	CHC***H***$_2$(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_2H	CD_3OD residual	5.82	m	CH	propylene
1.19	t, 7	CH_3	ethanol	3.31	s	NCH_3	dimethylacetamide	5.94	ddt	C***H***CH_2	allyl acetate
1.24	t, 7	CH_2CH_3	ethyl acetate	3.34	s	CH_3	methanol	5.94	ddt	C***H***CH_2	diallyl carbonate
1.29	br s	CH_2	H grease[g]	3.35	s	OCH_3	diglyme	6.08	m	CH(3,4)	pyrrole
1.29	m	CH_2	*n*-hexane	3.35	s	CH_3	1,2-dimethoxyethane	6.40	dd	CH(3,4)	furan
1.29	m	CH_2	*n*-pentane	3.44	s	CH_2	dimethyl malonate	6.71	s	ArH	BHA
1.29	br s	CH_2	pump oil	3.49	q, 7	CH_2	diethyl ether	6.72	m	CH(2,5)	pyrrole
1.34	sept, 7.3	CH_2	propane	3.52	s	CH_2	1,2-dimethoxyethane	6.92	s	ArH	BHT
1.40	s	CH_3	*tert*-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_3CO	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	C***H***$_2$CH$_3$	ethyl acetate	7.97	s	CH	dimethylformamide
2.07	s	CH_3CO	dimethylacetamide	4.34	s	CH_3	nitromethane	8.53	m	CH(2,6)	pyridine
2.12	s	CH_3CO	ethyl methyl ketone	4.56	ddd	CH_2	allyl acetate	10.00	s	HCO	benzaldehyde
2.15	s	CH_3	acetone								

Table S24. CD_3OD ($^{13}C\{^1H\}$ 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	($\mathbf{C}H_3$)$_3$C	BHA	64.71	CH	2-propanol	130.12	CH(3,5)	benzaldehyde
0.85	CH_3	acetonitrile	30.91	($\mathbf{C}H_3$)$_3$C	*tert*-butyl alcohol	66.14	CH_2	allyl acetate	130.64	CH(2,6)	benzaldehyde
1.99	CH_3	hexamethyldisiloxane	31.15	($\mathbf{C}H_3$)$_3$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	***C***HCH_2	diallyl carbonate
6.98	CH_3	ethane	31.61	CH_3	dimethylformamide	68.83	CH_2(2,5)	tetrahydrofuran	133.71	***C***HCH_2	allyl acetate
8.09	$CH_2\mathbf{C}H_3$	ethyl methyl ketone	32.73	CH_2(3,4)	*n*-hexane	69.35	CH_2	diallyl carbonate	134.61	CH	propylene
11.09	CH_3	triethylamine	35.30	CH_2(3)	*n*-pentane	69.40	(CH_3)$_3$***C***	*tert*-butyl alcohol	135.60	CH (4)	benzaldehyde
14.39	CH_3	*n*-pentane	35.36	(CH_3)$_3$***C***	BHT	71.33	CH_2	diglyme	136.31	CH(2)	imidazole
14.45	CH_3	*n*-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[i]	79.44	CH	chloroform	139.09	C(2,6)	BHT
16.90	CH_3	hexamethylbenzene	37.34	***C***H_2CH_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	***C***H_3CO	ethyl acetate	46.96	CH_2	triethylamine	118.22	CH***C***H_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_3Ar	BHT	49.00 (sept)	CD_3	CD_3OD signal	118.74	CH***C***H_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)	*n*-pentane	52.83	CH_3	dimethyl malonate	123.46	CH_2	ethylene	172.41	CO	allyl acetate
23.68	CH_2(2,5)	*n*-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_3O	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	C(4)	BHT	212.16	CO	ethyl methyl ketone
29.39	***C***H_3CO	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. D_2O (^1H NMR data by chemical shift in ppm)

shift	*mult*	*proton*	*impurity*	*shift*	*mult*	*proton*	*impurity*	*shift*	*mult*	*proton*	*impurity*
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_2O 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	CHC***H***$_2$(2)	allyl acetate
1.17	t, 7	CH_3	diethyl ether	3.07	m	CH_2(2,5)	pyrrolidine	5.32	ddt	CHC***H***$_2$(2)	diallyl carbonate
1.17	t, 7	CH_3	ethanol	3.18	q, 7	C***H***$_2$CH$_3$	ethyl methyl ketone	5.37	ddt	CHC***H***$_2$(1)	allyl acetate
1.17	d, 6	CH_3	2-propanol	3.34	s	CH_3	methanol	5.40	ddt	CHC***H***$_2$(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_2C***H***$_3$	ethyl acetate	3.37	s	CH_3	1,2-dimethoxyethane	5.90	m	CH	propylene
1.26	t, 7	CH_2C***H***$_3$	ethyl methyl ketone	3.56	q, 7	CH_2	diethyl ether	5.99	ddt	C***H***CH$_2$	allyl acetate
1.30	sept, 7.3	CH_2	propane	3.60	s	CH_2	1,2-dimethoxyethane	5.99	ddt	C***H***CH$_2$	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_3CO	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_2	1,4-dioxane	7.76–7.80	m	CH(4)	benzaldehyde
2.08	s	CH_3CO	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_3CO	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	C***H***$_2$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. D_2O ($^{13}C\{^1H\}$ NMR data by chemical shift in ppm)

shift	*carbon*	*impurity*	*shift*	*carbon*	*impurity*	*shift*	*carbon*	*impurity*	*shift*	*carbon*	*impurity*
1.47	CH_3	acetonitrile	36.46 (d)	CH_3	HMPA[i]	67.19	CH_2	1,4-dioxane	132.76	***C***HCH$_2$	diallyl carbonate
2.31	CH_3	hexamethyldisiloxane	37.27	***C***H$_2$CH$_3$	ethyl methyl ketone	68.68	CH_2(2,5)	tetrahydrofuran	134.70	CH (4)	benzaldehyde
7.87	CH$_2$***C***H$_3$	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	***C***H$_3$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	CH***C***H$_2$	diallyl carbonate	174.57	CO	dimethylacetamide
24.77	CH_2(4)	cyclohexanone	58.05	CH_2	ethanol	119.03	CH***C***H$_2$	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	***C***H$_3$CO	ethyl methyl ketone	63.17	CH_2	ethylene glycol	125.12	CH(3,5)	pyridine	197.25	CS_2	carbon disulfide
30.29	(***C***H$_3$)$_3$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	***C***HCH$_2$	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 $CDCl_3$, C_6D_6, $(CD_3)_2CO$, $(CD_3)_2SO$, CD_3CN, CD_3OD, and D_2O were previously reported in ref 1.

(3) A signal for HDO is also observed in $(CD_3)_2SO$ (3.30 ppm) and $(CD_3)_2CO$ (2.81 ppm), often seen as a 1:1:1 triplet ($^2J_{H,D}$ = 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 CH_2 and the OH protons may be observed (J = 5 Hz).

(7) In CD_3CN, the OH proton was seen as a multiplet at 2.69 ppm, as well as extra coupling to the CH_2 peak.

(8) Apiezon-brand H grease.

(9) In some solvents, the coupling interaction between the CH_3 and the OH protons may be observed (J = 5.5 Hz).

(10) Pyrrolidine was observed to react with the solvent $(CD_3)_2CO$.

(11) Phosphorus coupling was observed ($^2J_{PC}$ = 3 Hz).

(12) Internal reference; see Experimental Section in text.