APPENDIX C.

LISTING OF DETAILED MODEL SPECIES AND REACTIVITIES

This Appendix contains a complete listing and summary of all the detailed model species that are represented in the current mechanism, and gives the calculated reactivity results and the uncertainty assignments. Table C-1 lists all the detailed model species, indicates how they are represented in the model, gives their uncertainty classification and experimental availability codes, and other documentation notes and comments. It also gives the updated MIR values, calculated as discussed in Section VII, and the upper limit MIR values, derived as discussed in Appendix D. The uncertainty codes used in this table are defined in Table C-2, the experimental availability codes are defined in Table C-2, and the text for the comments footnotes is given in Table C-4. Table C-5 gives the compositions of the mixtures listed on Table C-1 whose reactivities are estimated, which were used as the basis for these estimates.

A summary of incremental and reactivity results using various scales in addition to MIR are given in Table C-6. The derivations of these scales are given in Section VII. This table includes averages of base case and adjusted NO_x reactivities calculated for the various 39 urban areas as discussed in Section VII. The reactivities calculated for the individual urban areas are given in Table C-7 and Table C-8, where the former has the O_3 yield reactivity data, and the latter has the reactivities relative to the maximum 8-hour average. Because of their length, Tables C-7 and C-8 are not included with the printed (or PDF) version of this report, but are available as supplementary material as Excel-97 files. They can be downloaded from a FTP site linked to http://cert.ucr.edu/~carter/reactdat.htm[1]

[1] This site may contain updated information when the mechanism and reactivity scale are updated in the future. However, it is expected that links and files will be retained so the version of the tables discussed in this report can still be downloaded.

Table C-1. Listing of detailed model species, their representation in the model, atmospheric reactivity estimates, and uncertainty assignments.

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]
CO	Carbon Monoxide	28.01	1	1	1,2	0.058	(0.45)	Expl
METHANE	Methane	16.04	1	4	1	0.0139	(0.025)	Asn'd
ETHANE	Ethane	30.07	1	2	1,2	0.31	(0.92)	Gen'd CH3-CH3
PROPANE	Propane	44.10	1	2	1,2,3	0.56	(2.61)	Gen'd CH3-CH2-CH3
N-C4	n-Butane	58.12	1	1	1,2,4	1.33	(4.00)	Gen'd CH3-CH2-CH2-CH3
N-C5	n-Pentane	72.15	1	7	4	1.54	(4.82)	Gen'd CH3-CH2-CH2-CH2-CH3
N-C6	n-Hexane	86.18	2	2	2,4	1.45	(5.08)	Gen'd CH3-CH2-CH2-CH2-CH2-CH3
N-C7	n-Heptane	100.21	2	-	4	1.28	(5.20)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH3
N-C8	n-Octane	114.23	2	1	2,4	1.11	(5.21)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C9	n-Nonane	128.26	3a	7	4	0.95	(5.02)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C10	n-Decane	142.29	3a	-	4	0.83	(4.82)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C11	n-Undecane	156.31	3a	-	4	0.74	(4.70)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C12	n-Dodecane	170.34	3a	1	2,4	0.66	(4.43)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C13	n-Tridecane	184.37	3a	-	4	0.62	(4.37)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C14	n-Tetradecane	198.40	3a	1	2,4	0.58	(4.23)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C15	n-Pentadecane	212.42	3a	1	2,4	0.56	(4.17)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C16	n-C16	226.45	3a	1	2,4	0.52	(4.04)	Gen'd CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
N-C17	n-C17	240.46	3a			0.49	(3.80)	L.Mol N-C16
N-C18	n-C18	254.49	3a			0.46	(3.57)	L.Mol N-C16
N-C19	n-C19	268.51	3a			0.44	(3.39)	L.Mol N-C16
N-C20	n-C20	282.54	3a			0.42	(3.22)	L.Mol N-C16
N-C21	n-C21	296.57	3a			0.40	(3.07)	L.Mol N-C16
N-C22	n-C22	310.59	3a			0.38	(2.93)	L.Mol N-C16
2-ME-C3	Isobutane	58.12	1	2	2,4,5	1.35	(3.63)	Gen'd CH3-CH(CH3)-CH3
2-ME-C4	Iso-Pentane	72.15	2	7	4	1.68	(4.52)	Gen'd CH3-CH(CH3)-CH2-CH3
22-DM-C3	Neopentane	72.15	2	7	3	0.69	(1.23)	Gen'd CH3-C(CH3)(CH3)-CH3
BR-C5	Branched C5 Alkanes	72.15	3	-	6	1.68	(4.52)	L.Mol 2-ME-C4
22-DM-C4	2,2-Dimethyl Butane	86.18	2	-	4	1.33	(2.61)	Gen'd CH3-C(CH3)(CH3)-CH2-CH3
23-DM-C4	2,3-Dimethyl Butane	86.18	2	7	4	1.14	(5.28)	Gen'd CH3-CH(CH3)-CH(CH3)-CH3
2-ME-C5	2-Methyl Pentane	86.18	2	-	4	1.80	(4.98)	Gen'd CH3-CH(CH3)-CH2-CH2-CH3
3-ME-C5	3-Methylpentane	86.18	2	-	4	2.07	(5.05)	Gen'd CH3-CH2-CH(CH3)-CH2-CH3
BR-C6	Branched C6 Alkanes	86.18	3	6	6	1.53	(5.15)	L.Mol 0.5 23-DM-C4 +0.25 3-ME-C5 +0.25 2-ME-C5
223TM-C4	2,2,3-Trimethyl Butane	100.21	2	-	4	1.32	(3.62)	Gen'd CH3-C(CH3)(CH3)-CH(CH3)-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
22-DM-C5	2,2-Dimethyl Pentane	100.21	2	-	4	1.22	(3.03)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH2-CH3
23-DM-C5	2,3-Dimethyl Pentane	100.21	2	-	4	1.55	(7.65)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH3
24-DM-C5	2,4-Dimethyl Pentane	100.21	2	-	4	1.65	(4.09)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH3
2-ME-C6	2-Methyl Hexane	100.21	2	-	4	1.37	(7.51)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH3
33-DM-C5	3,3-Dimethyl Pentane	100.21	2	-	3	1.32	(4.66)	Gen'd	CH3-CH2-C(CH3)(CH3)-CH2-CH3
3-ME-C6	3-Methyl Hexane	100.21	2	-	4	1.86	(7.65)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH3
BR-C7	Branched C7 Alkanes	100.21	3	-	6	1.63	(5.83)	L.Mol	0.5 24-DM-C5 +0.25 3-ME-C6 +0.25 2-ME-C6
2233M-C4	2,2,3,3-Tetramethyl Butane	114.23	3	-	4	0.44	(0.94)	Gen'd	CH3-C(CH3)(CH3)-C(CH3)(CH3)-CH3
224TM-C5	2,2,4-Trimethyl Pentane	114.23	2	2	2,4,5	1.44	(2.78)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH(CH3)-CH3
22-DM-C6	2,2-Dimethyl Hexane	114.23	3	-	4	1.13	(3.50)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH2-CH2-CH3
234TM-C5	2,3,4-Trimethyl Pentane	114.23	3	-	3	1.23	(4.61)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH(CH3)-CH3
23-DM-C6	2,3-Dimethyl Hexane	114.23	3	-	4	1.34	(7.23)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH2-CH3
24-DM-C6	2,4-Dimethyl Hexane	114.23	3	-	4	1.80	(7.23)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH3
25-DM-C6	2,5-Dimethyl Hexane	114.23	3	-	4	1.68	(7.13)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH(CH3)-CH3
2-ME-C7	2-Methyl Heptane	114.23	3	-	4	1.20	(7.13)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH3
3-ME-C7	3-Methyl Heptane	114.23	3	-	4	1.35	(7.23)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH3
4-ME-C7	4-Methyl Heptane	114.23	3	-	4	1.48	(7.23)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH3
BR-C8	Branched C8 Alkanes	114.23	3	-	6	1.57	(7.19)	L.Mol	0.5 24-DM-C6 +0.25 4-ME-C7 +0.25 2-ME-C7
225TM-C6	2,2,5-Trimethyl Hexane	128.26	3a	-	4	1.33	(5.56)	Gen'd	CH3-C(CH3)(CH3)-CH2-CH2-CH(CH3)-CH3
235TM-C6	2,3,5-Trimethyl Hexane	128.26	3a	-	4	1.33	(4.38)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH(CH3)-CH3
24-DM-C7	2,4-Dimethyl Heptane	128.26	3a	-	4	1.48	(6.80)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH3
2-ME-C8	2-Methyl Octane	128.26	3a	-	4	0.96	(5.05)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
33-DE-C5	3,3-Diethyl Pentane	128.26	3a	-	3	1.35	(3.15)	Gen'd	CH3-CH2-C(CH2-CH3)(CH2-CH3)-CH2-CH3
35-DM-C7	3,5-Dimethyl Heptane	128.26	3a	-	4	1.63	(6.87)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH3
4-ET-C7	4-Ethyl Heptane	128.26	3a	-	4	1.44	(6.87)	Gen'd	CH3-CH2-CH2-CH(CH2-CH3)-CH2-CH2-CH3
4-ME-C8	4-Methyl Octane	128.26	3a	-	4	1.08	(4.92)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH3
BR-C9	Branched C9 Alkanes	128.26	3a	-	6	1.25	(5.89)	L.Mol	0.5 24-DM-C7 +0.25 4-ME-C8 +0.25 2-ME-C8
24-DM-C8	2,4-Dimethyl Octane	142.29	3a	-	4	1.09	(6.38)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-CH3
26DM-C8	2,6-Dimethyl Octane	142.29	3a	1	2,4	1.27	(5.16)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH3
2-ME-C9	2-Methyl Nonane	142.29	3a	1	2,4	0.86	(5.13)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
34-DE-C6	3,4-Diethyl Hexane	142.29	3a	1a	2,4	1.20	(3.78)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH(CH2-CH3)-CH2-CH3
3-ME-C9	3-Methyl Nonane	142.29	3a	-	4	0.89	(6.38)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
4-ME-C9	4-Methyl Nonane	142.29	3a	-	4	0.99	(6.38)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH3
4-PR-C7	4-Propyl Heptane	142.29	3a	-	4	1.24	(6.44)	Gen'd	CH3-CH2-CH2-CH(CH2-CH2-CH3)-CH2-CH2-CH3
BR-C10	Branched C10 Alkanes	142.29	3a	6	6,7	1.09	(5.47)	L.Mol	0.5 26DM-C8 +0.25 4-ME-C9 +0.25 2-ME-C9
26DM-C9	2,6-Dimethyl Nonane	156.31	3a	-	4	0.95	(6.01)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
35-DE-C7	3,5-Diethyl Heptane	156.31	3a	-	4	1.21	(6.15)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C10	3-Methyl Decane	156.31	3a	-	4	0.77	(6.05)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
4-ME-C10	4-Methyl Decane	156.31	3a	-	4	0.80	(6.05)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
BR-C11	Branched C11 alkanes	156.31	3a	-	6,7	0.87	(6.01)	L.Mol	0.5 26DM-C9 +0.25 4-ME-C10 +0.25 3-ME-C10
36-DE-C8	2,6-Diethyl Octane	170.34	3a	-	4	1.09	(5.78)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH3
36DM-C10	3,6-Dimethyl Decane	170.34	3a	-	4	0.88	(5.72)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH3
3-ME-C11	3-Methyl Undecane	170.34	3a	-	4	0.70	(5.68)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
5-ME-C11	5-Methyl Undecane	170.34	3a	-	4	0.72	(5.68)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
BR-C12	Branched C12 Alkanes	170.34	3a	-	6,7	0.80	(5.72)	L.Mol	0.5 36DM-C10 +0.25 5-ME-C11 +0.25 3-ME-C11
36DM-C11	3,6-Dimethyl Undecane	184.37	3a	-	4	0.82	(5.42)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH3
37-DE-C9	3,7-Diethyl Nonane	184.37	3a	-	4	1.08	(5.48)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C12	3-Methyl Dodecane	184.37	3a	-	4	0.64	(5.38)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
5-ME-C12	5-Methyl Dodecane	184.37	3a	-	4	0.64	(5.38)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C13	Branched C13 Alkanes	184.37	3a	-	6,7	0.73	(5.42)	L.Mol	0.5 36DM-C11 +0.25 5-ME-C12 +0.25 3-ME-C12
37DM-C12	3,7-Dimethyl Dodecane	198.40	3a	-	4	0.74	(5.15)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH3
38DE-C10	3,8-Diethyl Decane	198.40	3a	-	4	0.68	(5.18)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C13	3-Methyl Tridecane	198.40	3a	-	4	0.57	(5.12)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
6-ME-C13	6-Methyl Tridecane	198.40	3a	-	4	0.62	(5.12)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C14	Branched C14 Alkanes	198.40	3a	-	6,7	0.67	(5.12)	L.Mol	0.5 37DM-C12 +0.25 6-ME-C13 +0.25 3-ME-C13
37DM-C13	3,7-Dimethyl Tridecane	212.42	3a	-	4	0.64	(4.88)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
39DE-C11	3,9-Diethyl Undecane	212.42	3a	-	4	0.62	(4.92)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH2-CH2-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH3
3-ME-C14	3-Methyl Tetradecane	212.42	3a	-	4	0.53	(4.85)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
6-ME-C14	6-Methyl Tetradecane	212.42	3a	-	4	0.57	(4.85)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C15	Branched C15 Alkanes	212.42	3a	-	6,7	0.60	(4.88)	L.Mol	0.5 37DM-C13 +0.25 6-ME-C14 +0.25 3-ME-C14
3-ME-C15	3-Methyl Pentadecane	226.45	3a	-	4	0.50	(4.65)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
48DM-C14	4,8-Dimethyl Tetradecane	226.45	3a	-	4	0.58	(4.65)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH3
7-ME-C15	7-Methyl Pentadecane	226.45	3a	-	4	0.51	(4.65)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
BR-C16	Branched C16 Alkanes	226.45	3a	-	6	0.54	(4.65)	L.Mol	0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
BR-C17	Branched C17 Alkanes	240.46	3a	-	6	0.51	(4.38)	L.Mol	0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
BR-C18	Branched C18 Alkanes	254.49	3a	-	6	0.48	(4.14)	L.Mol	0.5 48DM-C14 +0.25 7-ME-C15 +0.25 3-ME-C15
CYCC3	Cyclopropane	42.08	3	-	4	0.103	(0.21)	Gen'd	*CH2-CH2-CH2-*

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
CYCC4	Cyclobutane	56.11	3	-	3	1.05	(2.65)	Gen'd	*CH2-CH2-CH2-CH2-*
CYCC5	Cyclopentane	70.14	2	-	4	2.69	(5.92)	Gen'd	*CH2-CH2-CH2-CH2-CH2-*
CYCC6	Cyclohexane	84.16	2	1	2,4	1.46	(6.33)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CH2-*
IPR-CC3	Isopropyl Cyclopropane	84.16	3	-	4	1.52	(2.97)	Gen'd	*CH(CH(CH3)-CH3)-CH2-CH2-*
ME-CYCC5	Methylcyclopentane	84.16	3	-	4	2.42	(8.18)	Gen'd	*CH(CH3)-CH2-CH2-CH2-CH2-*
CYC-C6	C6 Cycloalkanes	84.16	3	6	6	1.46	(6.33)	L.Mol	CYCC6
13DMCYC5	1,3-Dimeth. Cyclopentane	98.19	3	-	4	2.15	(7.63)	Gen'd	*CH(CH3)-CH2-CH(CH3)-CH2-CH2-*
CYCC7	Cycloheptane	98.19	3	-	4	2.26	(7.46)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CH2-CH2-*
ET-CYCC5	Ethyl Cyclopentane	98.19	3	-	4	2.27	(7.87)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH2-CH2-*
ME-CYCC6	Methylcyclohexane	98.19	3	7	4	1.99	(6.54)	Gen'd	*CH(CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C7	C7 Cycloalkanes	98.19	3	-	6	1.99	(6.54)	L.Mol	ME-CYCC6
13DMCYC6	1,3-Dimethyl Cyclohexane	112.22	3	-	4	1.72	(8.21)	Gen'd	*CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-*
CYCC8	Cyclooctane	112.22	3	-	4	1.73	(6.78)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-*
ET-CYCC6	Ethylcyclohexane	112.22	3	-	4	1.75	(8.21)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
PR-CYCC5	Propyl Cyclopentane	112.22	3	-	4	1.91	(7.39)	Gen'd	*CH(CH2-CH2-CH3)-CH2-CH2-CH2-CH2-*
CYC-C8	C8 Cycloalkanes	112.22	3	-	6	1.75	(8.21)	L.Mol	ET-CYCC6
BCYC-C9	C9 Bicycloalkanes	124.23	3	-	6	1.57	(7.69)	L.Mol	0.5 C3-CYCC6 +0.5 1E4MCYC6
113MCYC6	1,1,3-Trimethyl Cyclohex.	126.24	3	-	4	1.37	(4.72)	Gen'd	*C(CH3)(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-*
1E4MCYC6	1-Eth.-4-Meth. Cyclohex.	126.24	3	-	4	1.62	(7.60)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C3-CYCC6	Propyl Cyclohexane	126.24	3	-	4	1.47	(7.56)	Gen'd	*CH(CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C9	C9 Cycloalkanes	126.24	3	-	6	1.55	(7.56)	L.Mol	0.5 C3-CYCC6 +0.5 1E4MCYC6
BCYC-C10	C10 Bicycloalkanes	138.25	3	-	6	1.29	(7.12)	L.Mol	0.34 C4-CYCC6 +0.33 1M3IPCY6 +0.33 14DECYC6
13DECYC6	1,3-Diethyl-Cyclohexane	140.27	3	-	4	1.34	(7.05)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH2-CH2-*
14DECYC6	1,4-Diethyl-Cyclohexane	140.27	3	-	4	1.49	(7.05)	Gen'd	*CH(CH2-CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH2-*
1M3IPCY6	1-Meth.-3-Isopr. Cyclohex.	140.27	3	-	4	1.26	(7.02)	Gen'd	*CH(CH(CH3)-CH3)-CH2-CH(CH3)-CH2-CH2-CH2-*
C4-CYCC6	Butyl Cyclohexane	140.27	3	-	4	1.07	(6.98)	Gen'd	*CH(CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C10	C10 Cycloalkanes	140.27	3	6	6,7	1.27	(7.02)	L.Mol	0.34 C4-CYCC6 +0.33 1M3IPCY6 +0.33 14DECYC6
BCYC-C11	C11 Bicycloalkanes	152.28	3	-	6	1.01	(6.62)	L.Mol	0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
13E5MCC6	13-Dieth-5-Me. Cyclohex.	154.30	3	-	4	1.11	(6.57)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH(CH3)-CH2-*
1E2PCYC6	1-Ethyl-2-Propyl Cyclohex.	154.30	3	-	4	0.95	(6.57)	Gen'd	*CH(CH2-CH3)-CH(CH2-CH2-CH3)-CH2-CH2-CH2-CH2-*
C5-CYCC6	Pentyl Cyclohexane	154.30	3	-	4	0.91	(6.50)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C11	C11 Cycloalkanes	154.30	3	-	6,7	0.99	(6.54)	L.Mol	0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
CYC-C11	C11 Cycloalkanes	154.30	3	-	6,7	0.99	(6.54)	L.Mol	0.34 C5-CYCC6 +0.33 13E5MCC6 +0.33 1E2PCYC6
BCYC-C12	C12 Bicycloalkanes	166.30	3	-	6	0.88	(5.82)	L.Mol	0.34 C6-CYCC6 +0.33 135ECYC6 +0.33 1M4C5CY6
CYC-C12	C12 Cycloalkanes	168.32	3	6	6,7	0.87	(5.75)	L.Mol	0.34 C6-CYCC6 +0.33 135ECYC6 +0.33 1M4C5CY6
135ECYC6	1,3,5-Triethyl Cyclohex.	168.33	3	-	4	1.06	(6.16)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-*

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1M4C5CY6	1-Meth.-4-Pentyl Cyclohex.	168.33	3	-	3	0.81	(6.09)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C6-CYCC6	Hexyl Cyclohexane	168.33	2	1	2,4	0.75	(4.96)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
BCYC-C13	C13 Bicycloalkanes	180.33	3	-	6	0.79	(5.81)	L.Mol	0.34 C7-CYCC6 +0.33 13E5PCC6 +0.33 1M2C6CC6
13E5PCC6	13-Dieth-5-Pent Cyclohx.	182.35	3	-	4	0.99	(5.78)	Gen'd	*CH(CH2-CH2-CH3)-CH2-CH(CH2-CH3)-CH2-CH(CH2-CH3)-CH2-*
1M2C6CC6	1-Meth.-2-Hexyl-Cyclohex.	182.35	3	-	4	0.70	(5.72)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH3)-CH(CH3)-CH2-CH2-CH2-CH2-*
C7-CYCC6	Heptyl Cyclohexane	182.35	3	-	4	0.66	(5.72)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C13	C13 Cycloalkanes	182.35	3	-	6,7	0.78	(5.75)	L.Mol	0.34 C7-CYCC6 +0.33 13E5PCC6 +0.33 1M2C6CC6
BCYC-C14	C14 Bicycloalkanes	194.36	3	6	6	0.71	(5.46)	L.Mol	0.34 C8-CYCC6 +0.33 13P5ECC6 +0.33 1M4C7CC6
13P5ECC6	13-Diprop-5-Eth Cyclohx.	196.38	3	-	4	0.94	(5.44)	Gen'd	*CH(CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-*
1M4C7CC6	1-Meth.-4-Heptyl Cyclohex.	196.38	3	-	3	0.58	(5.41)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C8-CYCC6	Octyl Cyclohexane	196.38	2	1	2,4	0.60	(5.37)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C14	C14 Cycloalkanes	196.38	3	-	6,7	0.71	(5.41)	L.Mol	0.34 C8-CYCC6 +0.33 13P5ECC6 +0.33 1M4C7CC6
BCYC-C15	C15 Bicycloalkanes	208.39	3	-	6	0.69	(5.18)	L.Mol	0.34 C9-CYCC6 +0.33 135PCYC6 +0.33 1M2C8CC6
135PCYC6	135-Tripropyl Cyclohex.	210.41	3	-	4	0.90	(5.17)	Gen'd	*CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-*
1M2C8CC6	1-Methyl-2-Octyl Cyclohex.	210.41	3	-	4	0.60	(5.10)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH(CH3)-CH2-CH2-CH2-CH2-*
C9-CYCC6	Nonyl Cyclohexane	210.41	3	-	4	0.54	(5.10)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C15	C15 Cycloalkanes	210.41	3	6	6,7	0.68	(5.13)	L.Mol	0.34 C9-CYCC6 +0.33 135PCYC6 +0.33 1M2C8CC6
13P5BCC6	1,3-Prop.-5-Butyl Cyclohex.	224.43	3	-	4	0.77	(4.89)	Gen'd	*CH(CH2-CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-CH(CH2-CH2-CH3)-CH2-*
1M4C9CY6	1-Methyl-4-Nonyl Cyclohex.	224.43	3	-	4	0.55	(4.86)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH(CH3)-CH2-CH2-*
C10CYCC6	Decyl Cyclohexane	224.43	3	-	4	0.50	(4.83)	Gen'd	*CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)-CH2-CH2-CH2-CH2-CH2-*
CYC-C16	C16 Cycloalkanes	224.43	3	6	6,7	0.61	(4.86)	L.Mol	0.34 C10CYCC6 +0.33 13P5BCC6 +0.33 1M4C9CY6
ETHENE	Ethene	28.05	1	1a	2,4	9.08	(19.51)	Gen'd	CH2=CH2
PROPENE	Propene	42.08	1	1	2,3,5	11.58	(23.89)	Gen'd	CH2=CH-CH3
1-BUTENE	1-Butene	56.11	2	3	2,4,5	10.29	(23.92)	Gen'd	CH2=CH-CH2-CH3
C4-OLE1	C4 Terminal Alkenes	56.11	2			10.29	(23.92)	L.Mol	1-BUTENE
1-PENTEN	1-Pentene	70.14	2	-	4	7.79	(23.92)	Gen'd	CH2=CH-CH2-CH2-CH3
3M-1-BUT	3-Methyl-1-Butene	70.14	3	-	4	6.99	(23.92)	Gen'd	CH2=CH-CH(CH3)-CH3
C5-OLE1	C5 Terminal Alkenes	70.14	2			7.79	(23.92)	L.Mol	1-PENTEN
1-HEXENE	1-Hexene	84.16	2	3	2,4,5	6.17	(19.95)	Gen'd	CH2=CH-CH2-CH2-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
33M1-BUT	3,3-Dimethyl-1-Butene	84.16	3	-	4	6.06	(19.88)	Gen'd	CH2=CH-C(CH3)(CH3)-CH3
3M1-C5E	3-Methyl-1-Pentene	84.16	3	-	4	6.22	(19.95)	Gen'd	CH2=CH-CH(CH3)-CH2-CH3
4M1-C5E	4-Methyl-1-Pentene	84.16	3	-	4	6.26	(19.95)	Gen'd	CH2=CH-CH2-CH(CH3)-CH3
C6-OLE1	C6 Terminal Alkenes	84.16	3			6.17	(19.95)	L.Mol	1-HEXENE
1-HEPTEN	1-Heptene	98.19	3	-	4	4.56	(17.11)	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH3
1-OCTENE	1-Octene	112.22	4	-	4	3.45	14.99	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH3
C8-OLE1	C8 Terminal Alkenes	112.22	4			3.45	14.99	L.Mol	1-OCTENE
1-C9E	1-Nonene	126.24	4	-	4	2.76	13.31	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C9-OLE1	C9 Terminal Alkenes	126.24	4			2.76	13.31	L.Mol	1-C9E
1-C10E	1-Decene	140.27	4	-	4	2.28	11.98	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C10-OLE1	C10 Terminal Alkenes	140.27	4			2.28	11.98	L.Mol	1-C10E
1-C11E	1-Undecene	154.30	4	-	4	1.95	10.88	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C11-OLE1	C11 Terminal Alkenes	154.30	4			1.95	10.88	L.Mol	1-C11E
C12-OLE1	C12 Terminal Alkenes	168.32	4			1.72	9.99	L.Mol	1-C12E
1-C12E	1-Dodecene	168.33	4	-	4	1.72	9.99	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
1-C13E	1-Tridecene	182.35	4	-	4	1.55	9.21	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C13-OLE1	C13 Terminal Alkenes	182.35	4			1.55	9.21	L.Mol	1-C13E
1-C14E	1-Tetradecene	196.38	4	-	4	1.48	8.56	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C14-OLE1	C14 Terminal Alkenes	196.38	4			1.48	8.56	L.Mol	1-C14E
1-C15E	1-Pentadecene	210.41	4	-	4	1.30	7.97	Gen'd	CH2=CH-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
C15-OLE1	C15 Terminal Alkenes	210.41	4			1.30	7.97	L.Mol	1-C15E
ISOBUTEN	Isobutene	56.11	1	2	2,4,5	6.35	(23.95)	Gen'd	CH2=C(CH3)-CH3
2M-1-BUT	2-Methyl-1-Butene	70.14	3	-	4	6.51	(23.95)	Gen'd	CH2=C(CH3)-CH2-CH3
23M1-BUT	23-Dimethyl-1-Butene	84.16	3	-	4	4.77	(19.95)	Gen'd	CH2=C(CH3)-CH(CH3)-CH3
2E1-BUT	2-Ethyl-1-Butene	84.16	3	-	4	5.04	(19.95)	Gen'd	CH2=C(CH2-CH3)-CH2-CH3
2M1-C5E	2-Methyl-1-Pentene	84.16	3	-	4	5.18	(19.95)	Gen'd	CH2=C(CH3)-CH2-CH2-CH3
233M1BUT	2,3,3-trimethyl-1-Butene	98.19	3	-	4	4.62	(17.11)	Gen'd	CH2=C(CH3)-C(CH3)(CH3)-CH3
C7-OLE1	C7 Terminal Alkenes	98.19	3			4.56	(17.11)	L.Mol	1-HEPTEN
3M2I1C4E	3-Methyl-2-Isopropyl-1-Butene	112.22	4	-	4	3.29	14.99	Gen'd	CH2=C(CH(CH3)-CH3)-CH(CH3)-CH3
C-2-BUTE	cis-2-Butene	56.11	2	7	3	13.22	(23.95)	Gen'd	CH3-CH=CH-CH3
T-2-BUTE	trans-2-Butene	56.11	1	1	2,3	13.91	(23.95)	Gen'd	CH3-CH=CH(CH3)
C4-OLE2	C4 Internal Alkenes	56.11	1			13.57	(23.95)	L.Mol	0.5 T-2-BUTE +0.5 C-2-BUTE
2M-2-BUT	2-Methyl-2-Butene	70.14	3	-	3	14.45	(23.95)	Gen'd	CH3-C(CH3)=CH-CH3
C-2-PENT	cis-2-Pentene	70.14	3	-	3	10.24	(23.95)	Gen'd	CH3-CH=CH-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
T-2-PENT	trans-2-Pentene	70.14	3	-	3	10.23	(23.95)	Gen'd	CH3-CH=CH(CH2-CH3)
2-C5-OLE	2-Pentenes	70.14	3			10.23	(23.95)	L.Mol	0.5 C-2-PENT +0.5 T-2-PENT
C5-OLE2	C5 Internal Alkenes	70.14	3			10.23	(23.95)	L.Mol	0.5 C-2-PENT +0.5 T-2-PENT
23M2-BUT	2,3-Dimethyl-2-Butene	84.16	3	-	3	13.32	(19.95)	Gen'd	CH3-C(CH3)=C(CH3)-CH3
2M-2-C5E	2-Methyl-2-Pentene	84.16	3	-	4	12.28	(19.95)	Gen'd	CH3-C(CH3)=CH-CH2-CH3
C-2-C6E	Cis-2-Hexene	84.16	3	-	4	8.44	(19.95)	Gen'd	CH3-CH=CH-CH2-CH2-CH3
C-3-C6E	Cis-3-Hexene	84.16	3	-	4	8.22	(19.95)	Gen'd	CH3-CH2-CH=CH-CH2-CH3
C3M2-C5E	Cis-3-Methyl-2-Hexene	84.16	3	-	4	13.38	(19.95)	Gen'd	CH3-CH=C(CH3)-CH2-CH3
T3M2-C5E	Trans 3-Methyl-2-Hexene	84.16	3	-	4	14.17	(19.95)	Gen'd	CH3-CH=C{CH3}-CH2-CH3
T4M2-C5E	Trans 4-Methyl-2-Hexene	84.16	3	-	4	7.88	(19.95)	Gen'd	CH3-CH(CH3)-CH=CH-CH3
T-2-C6E	Trans-2-Hexene	84.16	3	-	4	8.44	(19.95)	Gen'd	CH3-CH=CH(CH2-CH2-CH3)
T-3-C6E	Trans-3-Hexene	84.16	3	-	4	8.16	(19.95)	Gen'd	CH3-CH2-CH=CH(CH2-CH3)
2-C6-OLE	2-Hexenes	84.16	3			8.44	(19.95)	L.Mol	0.5 C-2-C6E +0.5 T-2-C6E
C6-OLE2	C6 Internal Alkenes	84.16	3			8.44	(19.95)	L.Mol	0.5 C-2-C6E +0.5 T-2-C6E
23M2-C5E	2,3-Dimethyl-2-Hexene	98.19	4	-	3	10.41	17.11	Gen'd	CH3-C(CH3)=C(CH3)-CH2-CH3
C-3-C7E	Cis-3-Heptene	98.19	4	-	4	6.96	17.11	Gen'd	CH3-CH2-CH=CH-CH2-CH2-CH3
T44M2C5E	Trans 4,4-dimethyl-2-Pentene	98.19	4	-	4	6.99	17.11	Gen'd	CH3-C(CH3)(CH3)-CH=CH-CH3
T-2-C7E	Trans-2-Heptene	98.19	4	-	4	7.33	17.11	Gen'd	CH3-CH=CH(CH2-CH2-CH2-CH3)
T-3-C7E	Trans-3-Heptene	98.19	4	-	4	6.96	17.11	Gen'd	CH3-CH2-CH=CH(CH2-CH2-CH3)
2-C7-OLE	2-Heptenes	98.19	3			6.96	(17.11)	L.Mol	0.5 T-3-C7E +0.5 C-3-C7E
C7-OLE2	C7 Internal Alkenes	98.19	3			6.96	(17.11)	L.Mol	T-3-C7E
C-4-C8E	Cis-4-Octene	112.22	4	-	4	5.94	14.99	Gen'd	CH3-CH2-CH2-CH=CH-CH2-CH2-CH3
T22M3C6E	Trans 2,2-Dimethyl 3-Hexene	112.22	4	-	4	5.97	14.99	Gen'd	CH3-C(CH3)(CH3)-CH=CH(CH2-CH3)
T25M3C6E	Trans 2,5-Dimethyl 3-Hexene	112.22	4	-	4	5.44	14.99	Gen'd	CH3-CH(CH3)-CH=CH(CH(CH3)-CH3)
T-3-C8E	Trans-3-Octene	112.22	4	-	4	6.13	14.99	Gen'd	CH3-CH2-CH=CH(CH2-CH2-CH2-CH3)
T-4-C8E	Trans-4-Octene	112.22	4	-	4	5.90	14.99	Gen'd	CH3-CH2-CH2-CH=CH(CH2-CH2-CH3)
3-C8-OLE	3-Octenes	112.22	4			6.13	14.99	L.Mol	T-3-C8E
C8-OLE2	C8 Internal Alkenes	112.22	4			5.90	14.99	L.Mol	T-4-C8E
244M2C5E	2,4,4-trimethyl-2-Pentene	126.24	4	-	4	5.85	13.32	Gen'd	CH3-C(CH3)=CH-C(CH3)(CH3)-CH2-CH3
3-C9-OLE	3-Nonenes	126.24	4			5.31	13.31	L.Mol	T-4-C9E
C9-OLE2	C9 Internal Alkenes	126.24	4			5.31	13.31	L.Mol	T-4-C9E
T-4-C9E	Trans-4-Nonene	128.26	4	-	4	5.23	13.10	Gen'd	CH3-CH2-CH2-CH=CH(CH2-CH2-CH2-CH3)
34E2-C6E	3,4-Diethyl-2-Hexene	140.27	4	-	4	3.95	11.98	Gen'd	CH3-CH=C(CH2-CH3)-CH(CH2-CH3)-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
C-5-C10E	Cis-5-Decene	140.27	4	-	4	4.89	11.98	Gen'd	CH3-CH2-CH2-CH2-CH=CH-CH2-CH2-CH2-CH3
T-4-C10E	Trans-4-Decene	140.27	4	-	4	4.50	11.98	Gen'd	CH3-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH3)
3C10-OLE	C10 3-Alkenes	140.27	4			4.50	11.98	L.Mol	T-4-C10E
C10-OLE2	C10 Internal Alkenes	140.27	4			4.50	11.98	L.Mol	T-4-C10E
T-5-C11E	Trans-5-Undecene	154.30	4	-	4	4.23	10.88	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH3)
3C11-OLE	C11 3-Alkenes	154.30	4			4.23	10.88	L.Mol	T-5-C11E
C11-OLE2	C11 Internal Alkenes	154.30	4			4.23	10.88	L.Mol	T-5-C11E
2C12-OLE	C12 2-Alkenes	168.32	4			3.75	9.99	L.Mol	T-5-C12E
3C12-OLE	C12 3-Alkenes	168.32	4			3.75	9.99	L.Mol	T-5-C12E
C12-OLE2	C12 Internal Alkenes	168.32	4			3.75	9.99	L.Mol	T-5-C12E
T-5-C12E	Trans-5-Dodecene	168.33	4	-	4	3.74	9.99	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH3)
T-5-C13E	Trans-5-Tridecene	182.35	4	-	4	3.38	9.21	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH2-CH3)
3C13-OLE	C13 3-Alkenes	182.35	4			3.38	9.21	L.Mol	T-5-C13E
C13-OLE2	C13 Internal Alkenes	182.35	4			3.38	9.21	L.Mol	T-5-C13E
T-5-C14E	Trans-5-Tetradecene	196.38	4	-	4	3.08	8.56	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)
3C14-OLE	C14 3-Alkenes	196.38	4			3.08	8.56	L.Mol	T-5-C14E
C14-OLE2	C14 Internal Alkenes	196.38	4			3.08	8.56	L.Mol	T-5-C14E
T-5-C15E	Trans-5-Pentadecene	210.41	4	-	4	2.82	7.97	Gen'd	CH3-CH2-CH2-CH2-CH=CH(CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3)
3C15-OLE	C15 3-Alkenes	210.41	4			2.82	7.97	L.Mol	T-5-C15E
C15-OLE2	C15 Internal Alkenes	210.41	4			2.82	7.97	L.Mol	T-5-C15E
C4-OLE	C4 Alkenes	56.11	4b	-	6	11.93	23.92	L.Mol	0.5 1-BUTENE +0.25 T-2-BUTE +0.25 C-2-BUTE
C5-OLE	C5 Alkenes	70.14	4b	-	6	9.01	23.92	L.Mol	0.5 1-PENTEN +0.25 C-2-PENT +0.25 T-2-PENT
C6-OLE	C6 Alkenes	84.16	4b	-	6	6.88	19.95	L.Mol	0.5 1-HEPTEN +0.25 C-2-C6E +0.25 T-2-C6E
C7-OLE	C7 Alkenes	98.19	4b	-	6	5.76	17.11	L.Mol	0.5 1-HEPTEN +0.5 T-3-C7E
C8-OLE	C8 Alkenes	112.22	4b	-	6	4.68	14.99	L.Mol	0.5 1-OCTENE +0.5 T-4-C8E
C9-OLE	C9 Alkenes	126.24	4b	-	6	4.03	13.31	L.Mol	0.5 1-C9E +0.5 T-4-C9E
C10-OLE	C10 Alkenes	140.27	4b	-	6	3.39	11.98	L.Mol	0.5 1-C10E +0.5 T-4-C10E
C11-OLE	C11 Alkenes	154.30	4b	-	6	3.09	10.88	L.Mol	0.5 1-C11E +0.5 T-5-C11E
C12-OLE	C12 Alkenes	168.32	4b	-	6	2.73	9.99	L.Mol	0.5 1-C12E +0.5 T-5-C12E
C13-OLE	C13 Alkenes	182.35	4b	-	6	2.46	9.21	L.Mol	0.5 1-C13E +0.5 T-5-C13E
C14-OLE	C14 Alkenes	196.38	4b	-	6	2.28	8.56	L.Mol	0.5 1-C14E +0.5 T-5-C14E
C15-OLE	C15 Alkenes	210.41	4b	-	6	2.06	7.97	L.Mol	0.5 1-C15E +0.5 T-5-C15E
CYC-PNTE	Cyclopentene	68.12	4	-	4	7.38	24.66	Gen'd	*CH=CH-CH2-CH2-CH2-*
1M-CC5E	1-Methyl cyclopentene	82.15	4	-	4	13.95	20.45	Gen'd	*C(CH3)=CH-CH2-CH2-CH2-*
CYC-HEXE	Cyclohexene	82.15	4	-	4	5.45	20.44	Gen'd	*CH=CH-CH2-CH2-CH2-CH2-*

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1M-CC6E	1-Methyl Cyclohexene	96.17	4	-	4	7.81	17.47	Gen'd	*C(CH3)=CH-CH2-CH2-CH2-CH2-*
4M-CC6E	4-Methyl Cyclohexene	96.17	4	-	4	4.48	17.47	Gen'd	*CH(CH3)-CH2-CH=CH-CH2-CH2-*
12M-CC6E	1,2-Dimethyl Cyclohexene	110.20	4	-	4	6.77	15.26	Gen'd	*C(CH3)=C(CH3)-CH2-CH2-CH2-CH2-*
13-BUTDE	1,3-Butadiene	54.09	3	-	4	13.58	(24.85)	Gen'd	CH2=CH-CH=CH2
ISOPRENE	Isoprene	68.12	1	1	2,3,5	10.69	(24.66)	Gen'd	CH2=CH-C(CH3)=CH2
C6-OL2D	C6 Cyclic or di-olefins	82.15	5b	-	6,8	8.65	20.44	L.Mol	0.5 C-2-C6E +0.5 T-2-C6E
C7-OL2D	C7 Cyclic or di-olefins	96.18	5b	-	6,8	7.49	17.47	L.Mol	T-2-C7E
C8-OL2D	C8 Cyclic or di-olefins	110.20	5b	-	6,8	6.01	15.26	L.Mol	T-4-C8E
C9-OL2D	C9 Cyclic or di-olefins	124.23	5b	-	6,8	5.40	13.53	L.Mol	T-4-C9E
C10-OL2D	C10 Cyclic or di-olefins	138.26	5b	-	6,8	4.56	12.15	L.Mol	T-4-C10E
C11-OL2D	C11 Cyclic or di-olefins	152.29	5b	-	6,8	4.29	11.03	L.Mol	T-5-C11E
C12-OL2D	C12 Cyclic or di-olefins	166.31	5b	-	6,8	3.79	10.11	L.Mol	T-5-C12E
C13-OL2D	C13 Cyclic or di-olefins	180.34	5b	-	6,8	3.42	9.31	L.Mol	T-5-C13E
C14-OL2D	C14 Cyclic or di-olefins	194.37	5b	-	6,8	3.11	8.64	L.Mol	T-5-C14E
C15-OL2D	C15 Cyclic or di-olefins	208.39	5b	-	6,8	2.85	8.05	L.Mol	T-5-C15E
CYC-PNDE	Cyclopentadiene	66.10	5	-	8	7.61	25.42	L.Mol	CYC-PNTE
3-CARENE	3-Carene	136.24	2c	3	2,9	3.21	(12.33)	Trp	
A-PINENE	a-Pinene	136.24	2c	1	2,9	4.29	(12.33)	Trp	
B-PINENE	b-Pinene	136.24	3c	1a	2,9	3.28	(12.33)	Trp	
D-LIMONE	d-Limonene	136.24	2c	3	2,9	3.99	(12.33)	Trp	
SABINENE	Sabinene	136.24	2c	3	2,9	3.67	(12.33)	Trp	
TERPENE	Terpene	136.24	4b	-	10	3.79	12.33	L.Mol	0.4 A-PINENE +0.25 B-PINENE +0.1 D-LIMONE +0.15 3-CARENE +0.1 SABINENE
STYRENE	Styrene	104.15	2	1	11	1.95	(16.15)	Asn'd	
AME-STYR	a-Methyl Styrene	118.18	4	-	8	1.72	14.22	L.Mol	STYRENE
C9-STYR	C9 Styrenes	118.18	4	-	8	1.72	14.22	L.Mol	STYRENE
C10-STYR	C10 Styrenes	132.21	4	-	8	1.53	12.71	L.Mol	STYRENE
BENZENE	Benzene	78.11	3c	1a	2,9	0.81	(4.39)	Asn'd	
TOLUENE	Toluene	92.14	2c	1	2,9	3.97	(12.07)	Asn'd	
C2-BENZ	Ethyl Benzene	106.17	2c	1	2,9	2.79	(11.54)	Asn'd	
I-C3-BEN	Isopropyl Benzene (cumene)	120.20	3c	-	8	2.32	(9.74)	Asn'd	
N-C3-BEN	n-Propyl Benzene	120.20	3c	-	8	2.20	(9.34)	Asn'd	
C9-BEN1	C9 Monosub. Benzenes	120.20	3c	-	8	2.20	(9.34)	L.Mol	N-C3-BEN
S-C4-BEN	s-Butyl Benzene	134.22	3c	-	8	1.97	(8.37)	Asn'd	
C10-BEN1	C10 Monosub. Benzenes	134.22	3c	-	8	1.97	(8.37)	L.Mol	N-C3-BEN

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
N-C4-BEN	n-Butyl Benzene	134.22	3c	-	8	1.97	(8.37)	L.Mol	N-C3-BEN
C11-BEN1	C11 Monosub. Benzenes	148.25	3c	-	8	1.78	(7.55)	L.Mol	N-C3-BEN
C12-BEN1	C12 Monosub. Benzenes	162.28	3c	-	8	1.63	(6.92)	L.Mol	N-C3-BEN
C13-BEN1	C13 Monosub. Benzenes	176.30	3c	-	8	1.50	(6.37)	L.Mol	N-C3-BEN
M-XYLENE	m-Xylene	106.17	2c	1	2,9	10.61	(15.62)	Asn'd	
O-XYLENE	o-Xylene	106.17	2c	1	2,9	7.49	(14.54)	Asn'd	
P-XYLENE	p-Xylene	106.17	2c	1	2,9	4.25	(14.68)	Asn'd	
C8-BEN2	C8 Disub. Benzenes	106.17	3b	6	6	5.16	(13.27)	L.Mol	0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C9-BEN2	C9 Disub. Benzenes	120.20	3b	-	6	6.61	(13.19)	L.Mol	0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C10-BEN2	C10 Disub. Benzenes	134.22	3b	-	6	5.92	(11.84)	L.Mol	0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C11-BEN2	C11 Disub. Benzenes	148.25	3b	-	6	5.35	(10.72)	L.Mol	0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C12-BEN2	C12 Disub. Benzenes	162.28	3b	-	6	4.90	(9.80)	L.Mol	0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C13-BEN2	C13 Disub. Benzenes	176.30	3b	-	6	4.50	(8.99)	L.Mol	0.34 M-XYLENE +0.33 O-XYLENE +0.33 P-XYLENE
C8-BEN2	Isomers of Ethylbenzene	106.17	4b	-	6	5.16	13.27	L.Mol	0.17 M-XYLENE +0.17 O-XYLENE+0.17 P-XYLENE +0.49 C2-BENZ
123-TMB	1,2,3-Trimethyl Benzene	120.20	2c	2	2,9	11.26	(13.94)	Asn'd	
124-TMB	1,2,4-Trimethyl Benzene	120.20	2c	2	2,9	7.18	(13.94)	Asn'd	
135-TMB	1,3,5-Trimethyl Benzene	120.20	2c	2	2,9	11.22	(13.98)	Asn'd	
C9-BEN	Isomers of Propylbenzene	120.20	4b	-	6	6.12	11.68	L.Mol	0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C9-BEN3	C9 Trisub. Benzenes	120.20	3b	6	6	9.90	(13.94)	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C10-BEN	Isomers of Butylbenzene	134.22	4b	-	6	5.48	10.48	L.Mol	0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C10-BEN4	C10 Tetrasub. Benzenes	134.22	4b	-	6	8.86	12.48	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C10-BEN3	C10 Trisub. Benzenes	134.22	3b	-	6	8.86	(12.48)	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11-BEN	Isomers of Pentylbenzene	148.25	4b	-	6	4.96	9.47	L.Mol	0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C11-BEN5	C11 Pentasub. Benzenes	148.25	4b	-	6	8.03	11.33	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11-BEN4	C11 Tetrasub. Benzenes	148.25	4b	-	6	8.03	11.33	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C11-BEN3	C11 Trisub. Benzenes	148.25	3b	-	6	8.03	(11.33)	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN	Isomers of Hexylbenzene	162.28	4b	-	6	4.53	8.66	L.Mol	0.17 135-TMB +0.17 123-TMB +0.17 124-TMB +0.49 N-C3-BEN
C12-BEN5	C11 Pentasub. Benzenes	162.28	4b	-	6	7.33	10.33	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN6	C12 Hexaasub. Benzenes	162.28	4b	-	6	7.33	10.33	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN4	C12 Tetrasub. Benzenes	162.28	4b	-	6	7.33	10.33	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C12-BEN3	C12 Trisub. Benzenes	162.28	3b	-	6	7.33	(10.33)	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
C13-BEN3	C13 Trisub. Benzenes	176.30	3b	-	6	6.75	(9.52)	L.Mol	0.34 135-TMB +0.33 123-TMB +0.33 124-TMB
INDAN	Indan	118.18	5c	-	8	3.17	14.18	L.Mol	TETRALIN
NAPHTHAL	Naphthalene	128.17	3c	3a,b	2,9	3.26	(12.85)	Asn'd	
TETRALIN	Tetralin	132.21	3c	3a	2,9	2.83	(12.67)	Asn'd	
ME-NAPH	Methyl Naphthalenes	142.20	3c	-a	9	4.61	(11.81)	Asn'd	

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1ME-NAPH	1-Methyl Naphthalene	142.20	3c	-	9	4.61	(11.81)	L.Mol	ME-NAPH
2ME-NAPH	2-Methyl Naphthalene	142.20	3c,h	-	9	4.61	(11.81)	L.Mol	ME-NAPH
C11-TET	C11 Tetralin or Indane	146.24	5c	-	8	2.56	11.48	L.Mol	TETRALIN
23-DMN	2,3-Dimethyl Naphth.	156.23	3c	3	2,9	5.54	(10.77)	Asn'd	
C12-NAP2	C12 Disub. Naphthalenes	156.23	3c	-	8	5.54	(10.77)	L.Mol	23-DMN
DM-NAPH	Dimethyl Naphthalenes	156.23	3c	-	8	5.54	(10.77)	L.Mol	23-DMN
C12-NAP1	C12 Monosub. Naphth.	156.23	3c	-	8	4.20	(10.77)	L.Mol	ME-NAPH
C13-NAP2	C13 Disub. Naphthalenes	170.26	4c	-	8	5.08	9.86	L.Mol	23-DMN
C13-NAP3	C13 Trisub. Naphthalenes	170.26	4c	-	8	5.08	9.86	L.Mol	23-DMN
C13-NAP1	C13 Monosub. Naphth.	170.26	4c	-	8	3.86	9.86	L.Mol	ME-NAPH
ACETYLEN	Acetylene	26.04	2	1	2,3,5	1.25	(3.98)	Gen'd	HC::CH
ME-ACTYL	Methyl Acetylene	40.07	4	-	3	6.45	16.64	Gen'd	HC::C-CH3
2-BUTYNE	2-Butyne	54.09	4	-	3	16.33	24.67	Gen'd	CH3-C::C-CH3
ET-ACTYL	Ethyl Acetylene	54.09	4	-	4	6.20	19.13	Gen'd	HC::C-CH2-CH3
MEOH	Methanol	32.04	1	2	2,3	0.71	(1.65)	Gen'd	CH3-OH
ETOH	Ethanol	46.07	1	2	2,3	1.69	(6.40)	Gen'd	CH3-CH2-OH
I-C3-OH	Isopropyl Alcohol	60.10	1	1	2,3	0.71	(7.14)	Gen'd	CH3-CH(OH)-CH3
N-C3-OH	n-Propyl Alcohol	60.10	2	-	4	2.74	(7.36)	Gen'd	CH3-CH2-CH2-OH
I-C4-OH	Isobutyl Alcohol	74.12	3	-	4	2.24	(10.18)	Gen'd	CH3-CH(CH3)-CH2-OH
N-C4-OH	n-Butyl Alcohol	74.12	3	-	4	3.34	(7.95)	Gen'd	CH3-CH2-CH2-CH2-OH
S-C4-OH	s-Butyl Alcohol	74.12	3	-	3	1.60	(11.73)	Gen'd	CH3-CH(OH)-CH2-CH3
T-C4-OH	t-Butyl Alcohol	74.12	3	1a	2,3,5	0.45	(1.54)	Gen'd	CH3-C(CH3)(OH)-CH3
CC5-OH	Cyclopentanol	86.13	3	-	4	1.96	(7.75)	Gen'd	*CH(OH)-CH2-CH2-CH2-CH2-*
2-C5OH	2-Pentanol	88.15	3	-	4	1.74	(7.95)	Gen'd	CH3-CH(OH)-CH2-CH2-CH3
3-C5OH	3-Pentanol	88.15	3	-	3	1.73	(8.09)	Gen'd	CH3-CH2-CH(OH)-CH2-CH3
C5OH	Pentyl Alcohol	88.15	3	-	4	3.35	(7.71)	Gen'd	CH3-CH2-CH2-CH2-CH2-OH
CC6-OH	Cyclohexanol	100.16	3	-	4	2.25	(10.18)	Gen'd	*CH(OH)-CH2-CH2-CH2-CH2-CH2-*
1-C6OH	1-Hexanol	102.18	3	-	4	2.74	(7.05)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-OH
2-C6OH	2-Hexanol	102.18	3	-	4	2.46	(6.93)	Gen'd	CH3-CH(OH)-CH2-CH2-CH2-CH3
1-C7OH	1-Heptanol	116.20	3	-	4	2.21	(6.48)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-OH
1-C8-OH	1-Octanol	130.23	2	1	2,4	2.01	(6.72)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-OH
2-ETC6OH	2-Ethyl-1-Hexanol	130.23	3	-	4	2.20	(7.28)	Gen'd	CH3-CH2-CH(CH2-OH)-CH2-CH2-CH2-CH3
2-C8-OH	2-Octanol	130.23	2	1	2,4	2.16	(7.20)	Gen'd	CH3-CH(OH)-CH2-CH2-CH2-CH2-CH2-CH3
3-C8-OH	3-Octanol	130.23	2	1	2,4	2.57	(7.64)	Gen'd	CH3-CH2-CH(OH)-CH2-CH2-CH2-CH2-CH3
4-C8-OH	4-Octanol	130.23	3	-	4	3.07	(7.46)	Gen'd	CH3-CH2-CH2-CH(OH)-CH2-CH2-CH2-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
I-C10-OH	8-Methyl-1-Nonanol (Isodecyl Alcohol)	158.29	3	-	4	1.18	(6.25)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-OH
ET-GLYCL	Ethylene Glycol	62.07	2	-	3	3.36	(10.10)	Gen'd	HO-CH2-CH2-OH
PR-GLYCL	Propylene Glycol	76.10	1	1	2,4	2.75	(11.71)	Gen'd	CH3-CH(OH)-CH2-OH
12-C4OH2	1,2-Butandiol	90.12	2	-	4	2.21	(11.06)	Gen'd	CH3-CH2-CH(OH)-CH2-OH
GLYCERL	Glycerol	92.10	2	-	4	3.27	(10.93)	Gen'd	HO-CH2-CH(OH)-CH2-OH
C6-GLYCL	1,2-Dihydroxy Hexane	118.18	3	-	4	2.75	(8.77)	Gen'd	CH3-CH2-CH2-CH2-CH(OH)-CH2-OH
2M24C5OH	2-Methyl-2,4-Pentanediol	118.18	3	-	4	1.04	(5.63)	Gen'd	CH3-C(CH3)(OH)-CH2-CH(OH)-CH3
ME-O-ME	Dimethyl Ether	46.07	1	2	2,3	0.93	(5.96)	Gen'd	CH3-O-CH3
TME-OX	Trimethylene Oxide	58.08	3	-	4	5.22	(11.26)	Gen'd	*CH2-CH2-CH2-O-*
THF	Tetrahydrofuran	72.11	3	-	4	4.95	(11.16)	Gen'd	*CH2-CH2-CH2-CH2-O-*
ET-O-ET	Diethyl Ether	74.12	2	1	2,3	4.01	(9.92)	Gen'd	CH3-CH2-O-CH2-CH3
METHYLAL	Dimethoxy methane	76.10	1	-	4	1.04	(5.32)	Gen'd	CH3-O-CH2-O-CH3
AM-THF	Alpha-Methyltetrahydro-furan	86.13	3	-	4	4.62	(10.42)	Gen'd	*CH(CH3)-CH2-CH2-CH2-O-*
THP	Tetrahydropyran	86.13	3	-	4	3.81	(8.75)	Gen'd	*CH2-CH2-CH2-CH2-CH2-O-*
ET-O-IPR	Ethyl Isopropyl Ether	88.15	3	-	3	3.86	(12.42)	Gen'd	CH3-CH(CH3)-O-CH2-CH3
MNBE	Methyl n-Butyl Ether	88.15	3	-	4	3.66	(8.82)	Gen'd	CH3-CH2-CH2-CH2-O-CH3
MTBE	Methyl t-Butyl Ether	88.15	1	2	2,3,5	0.78	(3.05)	Gen'd	CH3-C(CH3)(CH3)-O-CH3
PR-O-PR	Di n-Propyl Ether	102.18	3	-	4	3.24	(8.29)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-CH3
ENBE	Ethyl n-Butyl Ether	102.18	3	-	4	3.86	(8.71)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH3
ETBE	Ethyl t-Butyl Ether	102.18	3	8	3	2.11	(5.86)	Gen'd	CH3-C(CH3)(CH3)-O-CH2-CH3
MTAE	Methyl t-Amyl Ether	102.18	3	-	3	2.14	(5.50)	Gen'd	CH3-CH2-C(CH3)(CH3)-O-CH3
2BU-THF	2-Butyl Tetrahydrofuran	128.22	3	-	4	2.53	(8.72)	Gen'd	*CH(CH2-CH2-CH2-CH3)-CH2-CH2-CH2-O-*
IBU2-O	Di-Isobutyl Ether	130.23	3	-	3	1.29	(7.25)	Gen'd	CH3-CH(CH3)-CH2-O-CH2-CH(CH3)-CH3
BU-O-BU	Di-n-butyl Ether	130.23	3	-	4	3.17	(7.46)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-CH2-CH3
C5-O-C5	Di-n-Pentyl Ether	158.29	3	-	4	2.64	(6.43)	Gen'd	CH3-CH2-CH2-CH2-CH2-O-CH2-CH2-CH2-CH2-CH3
MEO-ETOH	2-Methoxyethanol	76.10	3	-	4	2.98	(9.75)	Gen'd	CH3-O-CH2-CH2-OH
MEOC3OH	1-Methoxy-2-Propanol	90.12	1	1	2,4,5	2.62	(9.65)	Gen'd	CH3-CH(OH)-CH2-O-CH3
ETO-ETOH	2-Ethoxyethanol	90.12	2	2	2,4,5	3.78	(9.44)	Gen'd	CH3-CH2-O-CH2-CH2-OH
2MEOC3OH	2-Methoxy-1-Propanol	90.12	3	-	4	3.01	(12.23)	Gen'd	CH3-O-CH(CH3)-CH2-OH
ETOC3OH	1-Ethoxy-2-Propanol	104.15	3	-	4	3.25	(10.65)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH3
2PROETOH	2-Propoxyethanol	104.15	3	-	4	3.52	(10.53)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-OH
3ETOC3OH	3-Ethoxy-1-Propanol	104.15	3	-	4	4.24	(8.62)	Gen'd	CH3-CH2-O-CH2-CH2-CH2-OH
3MEOC4OH	3-Methoxy-1-Butanol	104.15	3	-	4	0.97	(8.83)	Gen'd	CH3-O-CH(CH3)-CH2-CH2-OH
DET-GLCL	Diethylene Glycol	106.12	3	-	4	3.55	(10.53)	Gen'd	HO-CH2-CH2-O-CH2-CH2-OH

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
PROXC3OH	1-Propoxy-2-Propanol	118.18	3	-	4	2.86	(8.24)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH2-CH3
BUO-ETOH	2-Butoxyethanol	118.18	1	1	2,4,5	2.90	(7.97)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-OH
3MOMC4OH	3 methoxy -3 methyl-Butanol	118.18	3	-	4	1.74	(6.46)	Gen'd	CH3-O-C(CH3)(CH3)-CH2-CH2-OH
MOEOETOH	2-(2-Methoxyethoxy) Ethanol	120.15	3	-	4	2.90	(9.61)	Gen'd	CH3-O-CH2-CH2-O-CH2-CH2-OH
PG-1TB-E	1-tert-Butoxy-2-Propanol	132.20	3	-	4	1.71	(7.83)	Gen'd	CH3-C(CH3)(CH3)-O-CH2-CH(OH)-CH3
PG-2TB-E	2-tert-Butoxy-1-Propanol	132.20	3	-	4	1.81	(8.29)	Gen'd	CH3-C(CH3)(CH3)-O-CH(CH3)-CH2-OH
BUOC3OH	n-Butoxy-2-Propanol	132.20	3	-	4	2.70	(8.59)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH2-CH2-CH3
CARBITOL	2-(2-Ethoxyethoxy) EtOH	134.18	2	2	2,4,5	3.19	(8.22)	Gen'd	CH3-CH2-O-CH2-CH2-O-CH2-CH2-OH
DPR-GLCL	Dipropylene Glycol	134.18	3	-	4	2.48	(8.67)	Gen'd	CH3-CH(OH)-CH2-O-CH2-CH(OH)-CH3
EGHE	2-Hexyloxyethanol	146.23	3	-	3	2.45	(7.69)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-O-CH2-CH2-OH
DGPE	2-(2-Propoxyethoxy) ethanol	148.20	3	-	3	3.00	(8.00)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
DPRGOME	Dipropylene Glycol Methyl Ether	148.20	3	-	4	2.21	(8.07)	Gen'd	CH3-CH(OH)-CH2-O-CH(CH3)-CH2-O-CH3
C8-CELSV	2-(2-Butoxyethoxy)-EtOH	162.23	3	-	4	2.70	(7.31)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TGME	2-[2-(2-Methoxyethoxy) ethoxy] ethanol	164.20	3	-	3	2.62	(7.31)	Gen'd	CH3-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
EGEHE	2-(2-Ethylhexyloxy) ethanol	174.29	3	-	3	1.71	(6.58)	Gen'd	CH3-CH2-CH2-CH2-CH(CH2-CH3)-CH2-O-CH2-CH2-OH
TGEE	2-[2-(2-Ethoxyethoxy) ethoxy] ethanol	178.23	3	-	3	2.66	(6.77)	Gen'd	CH3-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
DGHE	2-(2-Hexyloxyethoxy) ethanol	190.29	3	-	3	2.03	(6.28)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TGPE	2-[2-(2-Propoxyethoxy) ethoxy] ethanol	192.26	3	-	3	2.46	(6.29)	Gen'd	CH3-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TGBE	2-[2-(2-Butoxyethoxy) ethoxy] ethanol	206.28	3	-	3	2.24	(5.86)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TPRGOME	Tripropylene Glycol Monomethyl Ether	206.28	3	-	4	1.90	(5.89)	Gen'd	CH3-CH(OH)-CH2-O-CH(CH3)-CH2-O-CH(CH3)-CH2-O-CH3
TETRAGME	2,5,8,11-Tetraoxatridecan-13-ol	208.26	3	-	3	2.15	(5.83)	Gen'd	CH3-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
TETRAGBE	3,6,9,12-Tetraoxahexadecan-1-ol	250.34	3	-	3	1.90	(4.86)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CH2-CH2-OH
ME-FORM	Methyl Formate	60.05	3	-	3	0.066	(0.46)	Gen'd	CH3-O-CHO

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
ET-FORM	Ethyl Formate	74.08	3	-	3	0.52	(1.92)	Gen'd	CH3-CH2-O-CHO
ME-ACET	Methyl Acetate	74.08	1	1	2,3,5	0.073	(0.68)	Gen'd	CH3-O-CO-CH3
ET-ACET	Ethyl Acetate	88.11	1	1	2,4,5	0.64	(2.46)	Gen'd	CH3-CH2-O-CO-CH3
ME-PRAT	Methyl Propionate	88.11	3	-	4	0.71	(1.63)	Gen'd	CH3-CH2-CO-O-CH3
C3-FORM	n-Propyl Formate	88.11	3	-	4	0.93	(3.51)	Gen'd	CH3-CH2-CH2-O-CHO
ET-PRAT	Ethyl Propionate	102.13	3	-	4	0.79	(2.75)	Gen'd	CH3-CH2-O-CO-CH2-CH3
IPR-ACET	Isopropyl Acetate	102.13	2	2	2,4	1.24	(4.09)	Gen'd	CH3-CH(CH3)-O-CO-CH3
ME-BUAT	Methyl Butyrate	102.13	3	-	4	1.18	(3.74)	Gen'd	CH3-CH2-CH2-CO-O-CH3
ME-IBUAT	Methyl Isobutyrate	102.13	2	1	2,4,5	0.70	(2.28)	Gen'd	CH3-CH(CH3)-CO-O-CH3
C4-FORM	n-Butyl Formate	102.13	3	-	4	0.95	(3.81)	Gen'd	CH3-CH2-CH2-CH2-O-CHO
PR-ACET	Propyl Acetate	102.13	3	-	4	0.87	(4.09)	Gen'd	CH3-CH2-CH2-O-CO-CH3
ET-BUAT	Ethyl Butyrate	116.16	3	-	4	1.25	(4.84)	Gen'd	CH3-CH2-CH2-CO-O-CH2-CH3
IBU-ACET	Isobutyl Acetate	116.16	3	-	3	0.67	(7.31)	Gen'd	CH3-CH(CH3)-CH2-O-CO-CH3
ME-PVAT	Methyl Pivalate	116.16	2	1	2,3,5	0.41	(1.51)	Gen'd	CH3-C(CH3)(CH3)-CO-O-CH3
BU-ACET	n-Butyl Acetate	116.16	2	1	2,4,5	0.89	(4.26)	Gen'd	CH3-CH2-CH2-CH2-O-CO-CH3
PR-PRAT	n-Propyl Propionate	116.16	3	-	4	0.93	(4.12)	Gen'd	CH3-CH2-CH2-O-CO-CH2-CH3
SBU-ACET	s-Butyl Acetate	116.16	3	-	3	1.43	(5.23)	Gen'd	CH3-CH2-CH(CH3)-O-CO-CH3
TBU-ACET	t-Butyl Acetate	116.16	2	1	2,4,5	0.22	(0.53)	Gen'd	CH3-C(CH3)(CH3)-O-CO-CH3
BU-PRAT	Butyl Propionate	130.19	3	-	4	0.89	(6.89)	Gen'd	CH3-CH2-CH2-CH2-O-CO-CH2-CH3
AM-ACET	Amyl Acetate	130.19	3	-	4	0.96	(7.56)	Gen'd	CH3-CH2-CH2-CH2-CH2-O-CO-CH3
PR-BUAT	n-Propyl Butyrate	130.19	3	-	4	1.17	(5.73)	Gen'd	CH3-CH2-CH2-O-CO-CH2-CH2-CH3
23MC4ACT	2,3-Dimethylbutyl Acetate	144.22	3	-	3	0.84	(10.97)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
2MC5-ACT	2-Methylpentyl Acetate	144.22	3	-	3	1.11	(10.97)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
3MC5-ACT	3-Methylpentyl Acetate	144.22	3	-	3	1.31	(10.97)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
4MC5-ACT	4-Methylpentyl Acetate	144.22	3	-	3	0.92	(10.89)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
IBU-IBTR	Isobutyl Isobutyrate	144.22	3	-	3	0.64	(6.52)	Gen'd	CH3-CH(CH3)-CH2-O-CO-CH(CH3)-CH3
BU-BUAT	n-Butyl Butyrate	144.22	3	-	4	1.12	(6.36)	Gen'd	CH3-CH2-CH2-CH2-O-CO-CH2-CH2-CH3
NC6-ACET	n-Hexyl Acetate	144.22	3	-	3	0.87	(10.89)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
E3EOC3OH	Ethyl 3-Ethoxy Propionate	146.19	3	-	4	3.61	(10.07)	Gen'd	CH3-CH2-O-CH2-CH2-CO-O-CH2-CH3
24MC5ACT	2,4-Dimethylpentyl Acetate	158.24	3	-	3	0.98	(10.24)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
2MC6-ACT	2-Methylhexyl Acetate	158.24	3	-	3	0.89	(10.24)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
3EC5-ACT	3-Ethylpentyl Acetate	158.24	3	-	3	1.24	(10.29)	Gen'd	CH3-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
3MC6-ACT	3-Methylhexyl Acetate	158.24	3	-	3	1.01	(10.24)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
4MC6-ACT	4-Methylhexyl Acetate	158.24	3	-	3	0.91	(10.24)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
5MC6-ACT	5-Methylhexyl Acetate	158.24	3	-	3	0.79	(10.21)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH2-CH2-O-CO-CH3
IC5IBUAT	Isoamyl Isobutyrate	158.24	3	-	4	0.89	(6.63)	Gen'd	CH3-CH(CH3)-CH2-CH2-O-CO-CH(CH3)-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
NC7-ACET	n-Heptyl Acetate	158.24	3	-	3	0.73	(10.21)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
24MC6ACT	2,4-Dimethylhexyl Acetate	172.27	3	-	3	0.93	(9.56)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
2ETHXACT	2-Ethyl-Hexyl Acetate	172.27	3	-	4	0.79	(7.27)	Gen'd	CH3-CH2-CH2-CH2-CH(CH2-CH3)-CH2-O-CO-CH3
34MC6ACT	3,4-Dimethylhexyl Acetate	172.27	3	-	3	1.16	(9.56)	Gen'd	CH3-CH2-CH(CH3)-CH(CH3)-CH2-CH2-O-CO-CH3
35MC6ACT	3,5-Dimethylhexyl Acetate	172.27	3	-	3	1.09	(9.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3EC6-ACT	3-Ethylhexyl Acetate	172.27	3	-	3	1.03	(9.59)	Gen'd	CH3-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
3MC7-ACT	3-Methylheptyl Aceate	172.27	3	-	3	0.76	(9.56)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
45MC6ACT	4,5-Dimethylhexyl Acetate	172.27	3	-	3	0.86	(9.56)	Gen'd	CH3-CH(CH3)-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
4MC7-ACT	4-Methylheptyl Acetate	172.27	3	-	3	0.72	(9.56)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
5MC7-ACT	5-Methylheptyl Aceate	172.27	3	-	3	0.73	(9.56)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH2-CH2-O-CO-CH3
NC8-ACET	n-Octyl Acetate	172.27	3	-	3	0.64	(9.53)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
235M6ACT	2,3,5-Teimethylhexyl Acetate	186.30	3	-	3	0.86	(8.93)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
23MC7ACT	2,3-Dimethylheptyl Acetate	186.30	3	-	3	0.84	(8.93)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
24MC7ACT	2,4-Dimethylheptyl Acetate	186.30	3	-	3	0.88	(8.93)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
25MC7ACT	2,5-Dimethylheptyl Acetate	186.30	3	-	3	0.86	(8.93)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
2MC8-ACT	2-Methyloctyl Acetate	186.30	3	-	3	0.63	(8.90)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH(CH3)-CH2-O-CO-CH3
35MC7ACT	3,5-Dimethylheptyl Acetate	186.30	3	-	3	1.01	(8.93)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
36MC7ACT	3,6-Dimethylheptyl Acetate	186.30	3	-	3	0.87	(8.90)	Gen'd	CH3-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3EC7-ACT	3-Ethylheptyl Acetate	186.30	3	-	3	0.71	(8.93)	Gen'd	CH3-CH2-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
45MC7ACT	4,5-Dimethylheptyl Acetate	186.30	3	-	3	0.96	(8.93)	Gen'd	CH3-CH2-CH(CH3)-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
46MC7ACT	4,6-Dimethylheptyl Acetate	186.30	3	-	3	0.83	(8.90)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
4MC8-ACT	4-Methyloctyl Acetate	186.30	3	-	3	0.68	(8.90)	Gen'd	CH3-CH2-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
5MC8-ACT	5-Methyloctyl Acetate	186.30	3	-	3	0.67	(8.90)	Gen'd	CH3-CH2-CH2-CH(CH3)-CH2-CH2-CH2-CH2-O-CO-CH3
NC9-ACET	n-Nonyl Acetate	186.30	3	-	3	0.58	(8.90)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH2-O-CO-CH3
36MC8ACT	3,6-Dimethyloctyl Acetate	200.32	3	-	3	0.88	(8.34)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3IPC7ACT	3-Isopropylheptyl Acetate	200.32	3	-	3	0.71	(8.34)	Gen'd	CH3-CH2-CH2-CH2-CH(CH(CH3)-CH3)-CH2-CH2-O-CO-CH3
46MC8ACT	4,6-Dimethyloctyl Acetate	200.32	3	-	3	0.85	(8.34)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
357M8ACT	3,5,7-Trimethyloctyl Acetate	214.35	3	-	3	0.83	(7.80)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
3E6M8ACT	3-Ethyl-6-Methyloctyl Acetate	214.35	3	-	3	0.80	(7.80)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
47MC9ACT	4,7-Dimethylnonyl Acetate	214.35	3	-	3	0.64	(7.80)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
2357M8AC	2,3,5,7-Tetramethyloctyl Acetate	228.38	3	-	3	0.74	(7.36)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
357M9ACT	3,5,7-Trimethylnonyl Acetate	228.38	3	-	3	0.76	(7.36)	Gen'd	CH3-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
368M9ACT	3,6,8-Trimethylnonyl Acetate	228.38	3	-	3	0.72	(7.33)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
2468M8AC	2,4,6,8-Tetramethylnonyl Acetate	242.41	3	-	3	0.63	(6.92)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-O-CO-CH3
3E67M9AC	3-Ethyl-6,7-Dimethylnonyl Acetate	242.41	3	-	3	0.76	(6.92)	Gen'd	CH3-CH2-CH(CH3)-CH(CH3)-CH2-CH2-CH(CH2-CH3)-CH2-CH2-O-CO-CH3
479M10AC	4,7,9-Trimethyldecyl Acetate	242.41	3	-	3	0.55	(6.92)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH2-CH(CH3)-CH2-CH2-CH2-O-CO-CH3
23568M9A	2,3,5,6,8-Pentaamethylnonyl Acetate	256.43	3	-	3	0.74	(6.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-CH(CH3)-CH(CH3)-CH2-O-CO-CH3
3579M10A	3,5,7,9-Tetramethyldecyl Acetate	256.43	3	-	3	0.58	(6.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
5E368M9A	5-Ethyl-3,6,8-Trimethylnonyl Acetate	256.43	3	-	3	0.77	(6.56)	Gen'd	CH3-CH(CH3)-CH2-CH(CH3)-CH(CH2-CH3)-CH2-CH(CH3)-CH2-CH2-O-CO-CH3
DMC	Dimethyl Carbonate	90.08	2	1	2,3	0.059	(0.53)	Gen'd	CH3-O-CO-O-CH3
PC	Propylene Carbonate	102.09	2	1	2,4,5	0.25	(0.96)	Gen'd	*CH(CH3)-CH2-O-CO-O-*
ME-LACT	Methyl Lactate	104.11	3	-	4	2.75	(3.38)	Gen'd	CH3-CH(OH)-CO-O-CH3
MCSVACET	2-Methoxyethyl Acetate	118.13	3	-	3	1.18	(11.07)	Gen'd	CH3-O-CH2-CH2-O-CO-CH3
ET-LACT	Ethyl Lactate	118.13	3	-	4	2.71	(3.96)	Gen'd	CH3-CH(OH)-CO-O-CH2-CH3
MIPR-CB	Methyl Isopropyl Carbonate	118.13	2	1	2,3,5	0.69	(2.78)	Gen'd	CH3-CH(CH3)-O-CO-O-CH3
PGME-ACT	1-Methoxy-2-Propyl Acetate	132.16	2	1	2,4	1.71	(8.09)	Gen'd	CH3-O-CH2-CH(CH3)-O-CO-CH3
CSV-ACET	2-Ethoxyethyl Acetate	132.16	3	-	4	1.90	(11.09)	Gen'd	CH3-CH2-O-CH2-CH2-O-CO-CH3
2PGMEACT	2-Methyoxy-1-propyl Acetate	132.16	3	-	3	1.12	(11.53)	Gen'd	CH3-O-CH(CH3)-CH2-O-CO-CH3
DBE-4	Dimethyl Succinate	146.14	3	1a	2,4,5	0.25	(1.40)	Gen'd	CH3-O-CO-CH2-CH2-CO-O-CH3
ETGLDACT	Ethylene Glycol Diacetate	146.14	3	-	3	0.72	(5.16)	Gen'd	CH3-CO-O-CH2-CH2-O-CO-CH3
DIPR-CB	Diisopropyl Carbonate	146.19	3	-	4	1.04	(7.15)	Gen'd	CH3-CH(CH3)-O-CO-O-CH(CH3)-CH3
DBE-5	Dimethyl Glutarate	160.17	3	1a	2,4,5	0.49	(2.66)	Gen'd	CH3-O-CO-CH2-CH2-CH2-CO-O-CH3
2BUETACT	2-Butoxyethyl Acetate	160.21	3	-	4	1.67	(9.59)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CO-CH3
DBE-6	Dimethyl Adipate	174.20	3	-	4	1.95	(4.76)	Gen'd	CH3-O-CO-CH2-CH2-CH2-CH2-CO-O-CH3
DGEEA	2-(2-Ethoxyethoxy) ethyl acetate	176.21	3	-	3	1.50	(9.41)	Gen'd	CH3-CH2-O-CH2-CH2-O-CH2-CH2-O-CO-CH3

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
DGBEA	2-(2-Butoxyethoxy) ethyl acetate	204.27	3	-	3	1.38	(8.22)	Gen'd	CH3-CH2-CH2-CH2-O-CH2-CH2-O-CH2-CH2-O-CO-CH3
SC7ESC12	Substituted C7 ester (C12)	211.19	4	-	12	0.92	6.52	L.Mol	0.67 TEXANOL1 +0.33 TEXANOL2
TEXANOL2	1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	216.32	3	-	4	0.92	(6.10)	Gen'd	CH3-CH(CH3)-CO-O-CH(CH(CH3)-CH3)-C(CH3)(CH3)-CH2-OH
TEXANOL1	3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	216.32	3	-	4	0.88	(6.50)	Gen'd	CH3-CH(CH3)-CH(OH)-C(CH3)(CH3)-CH2-O-CO-CH(CH3)-CH3
TEXANOL	Texanol isomers	216.32	3	-	13	0.89	(6.36)	L.Mol	0.67 TEXANOL1 +0.33 TEXANOL2
SC9ESC12	Substituted C9 Ester (C12)	218.24	4	-	12	0.89	6.31	L.Mol	0.67 TEXANOL1 +0.33 TEXANOL2
ETOX	Ethylene Oxide	44.05	3	-	3	0.045	(0.185)	Gen'd	*CH2-CH2-O-*
PROX	Propylene Oxide	58.08	3	-	3	0.32	(0.94)	Gen'd	*CH(CH3)-CH2-O-*
12BUOX	1,2-Epoxybutane	72.11	3	-	3	1.02	(2.56)	Gen'd	*CH(CH2-CH3)-CH2-O-*
FORMACID	Formic Acid	46.03	3	-	3	0.076	(0.58)	Gen'd	HCO-OH
ACETACID	Acetic Acid	60.05	3	-	4	0.71	(1.37)	Gen'd	CH3-CO-OH
ACYRACID	Acrylic Acid	72.06	5	-	4	11.66	13.97	Gen'd	CH2=CH-CO-OH
PROPACID	Propionic Acid	74.08	3	-	4	1.16	(1.58)	Gen'd	CH3-CH2-CO-OH
ME-ACRYL	Methyl Acrylate	86.09	5	-	4	12.24	15.61	Gen'd	CH2=CH-CO-O-CH3
VIN-ACET	Vinyl Acetate	86.09	5	-	4	3.26	15.61	Gen'd	CH2=CH-O-CO-CH3
MBUTENOL	2-Methyl-2-Butene-3-ol	86.13	3	-	4	4.12	(15.60)	Gen'd	CH2=CH-C(CH3)(OH)-CH3
ET-ACRYL	Ethyl Acrylate	100.11	5	-	4	8.78	16.78	Gen'd	CH2=CH-CO-O-CH2-CH3
ME-MACRT	Methyl Methacrylate	100.12	5	-	3	15.84	16.78	Gen'd	CH2=C(CH3)-CO-O-CH3
BU-MACRT	Butyl Methacrylate	142.20	5	-	3	9.09	11.83	Gen'd	CH2=C(CH3)-CO-O-CH2-CH2-CH2-CH3
IBUMACRT	Isobutyl Methacrylate	142.20	5	-	3	8.99	11.83	Gen'd	CH2=C(CH3)-CO-O-CH2-CH(CH3)-CH3
FURAN	Furan	68.08	4	3c	8	16.54	24.37	L.Mol	M-XYLENE
FORMALD	Formaldehyde	30.03	2a	1	1,2,14	8.97	(15.81)	Expl	
ACETALD	Acetaldehyde	44.05	1	1	1,2,14	6.84	(21.36)	Expl	
PROPALD	Propionaldehyde	58.08	2	7	14	7.89	(24.64)	Expl	
2MEC3AL	2-Methylpropanal	72.11	3	-	3	5.87	(26.57)	Gen'd	CH3-CH(CHO)-CH3
1C4RCHO	Butanal	72.11	3	-	4	6.74	(26.55)	Gen'd	CH3-CH2-CH2-CHO
C4-RCHO	C4 aldehydes	72.11	3			6.74	(26.55)	L.Mol	1C4RCHO
22DMC3AL	2,2-Dimethylpropanal (pivaldehyde)	86.13	3	-	3	5.40	(22.24)	Gen'd	CH3-C(CH3)(CHO)-CH3
3MC4RCHO	3-Methylbutanal (Isovaleraldehyde)	86.13	3	-	4	5.52	(22.26)	Gen'd	CH3-CH(CH3)-CH2-CHO

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
1C5RCHO	Pentanal (Valeraldehyde)	86.13	3	-	4	5.76	(22.26)	Gen'd	CH3-CH2-CH2-CH2-CHO
C5-RCHO	C5 Aldehydes	86.14	3			5.76	(22.26)	L.Mol	1C5RCHO
GLTRALD	Glutaraldehyde	100.12	3	-	3	4.79	(19.18)	Gen'd	HCO-CH2-CH2-CH2-CHO
1C6RCHO	Hexanal	100.16	3	-	4	4.98	(19.18)	Gen'd	CH3-CH2-CH2-CH2-CH2-CHO
C6-RCHO	C6 Aldehydes	100.16	3			4.98	(19.18)	L.Mol	1C6RCHO
1C7RCHO	Heptanal	114.19	3	-	4	4.23	(16.80)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CHO
C7-RCHO	C7 Aldehydes	114.19	3			4.23	(16.80)	L.Mol	1C7RCHO
1C8RCHO	Octanal	128.22	3	-	4	3.65	(14.97)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CHO
C8-RCHO	C8 Aldehydes	128.22	3			3.65	(14.97)	L.Mol	1C8RCHO
GLYOXAL	Glyoxal	58.04	3	5	5,14	14.22	(16.54)	Expl	
MEGLYOX	Methyl Glyoxal	72.07	3	-	14	16.21	(19.98)	Expl	
ACROLEIN	Acrolein	56.06	3	3a	2,4,5	7.60	(25.69)	Gen'd	CH2=CH-CHO
CROTALD	Crotonaldehyde	70.09	3	-	4	10.07	(27.39)	Gen'd	CH3-CH=CH(CHO)
METHACRO	Methacrolein	70.09	1	3	2,5,14	6.23	(27.39)	Gen'd	CH2=C(CHO)-CH3
HOMACR	Hydroxy Methacrolein	86.09	3	-	4	6.61	(22.30)	Gen'd	CH2=C(CHO)-CH2-OH
BENZALD	Benzaldehyde	106.13	2			-0.61	(18.08)	Expl	
TOLUALD	Tolualdehyde	120.15	3			-0.54	(15.98)	L.Mol	BENZALD
ACETONE	Acetone	58.08	1			0.43	(8.28)	Expl	
CC4-KET	Cyclobutanone	70.09	4	-	3	0.68	11.40	Gen'd	*CH2-CH2-CH2-CO-*
MEK	Methyl Ethyl Ketone	72.11	1	1	2,3,5	1.49	(11.96)	Gen'd	CH3-CH2-CO-CH3
CC5-KET	Cyclopentanone	84.12	4	-	4	1.43	13.69	Gen'd	*CH2-CH2-CH2-CH2-CO-*
KET5C	C5 Cyclic Ketones	84.12	4b	-	8	1.43	13.69	L.Mol	CC5-KET
MPK	2-Pentanone	86.13	2	1	2,4,5	3.07	(15.69)	Gen'd	CH3-CH2-CH2-CO-CH3
DEK	3-Pentanone	86.13	3	-	4	1.45	(11.70)	Gen'd	CH3-CH2-CO-CH2-CH3
KET5	C5 Ketones	86.13	3	-	8	3.07	(15.69)	L.Mol	MPK
CC6-KET	Cyclohexanone	98.15	3	1a	2,4,5	1.61	(15.40)	Gen'd	*CH2-CH2-CH2-CH2-CH2-CO-*
KET6C	C6 Cyclic Ketones	98.15	4b	-	8	1.61	15.40	L.Mol	CC6-KET
MIBK	4-Methyl-2-Pentanone	100.16	2	1	2,4,5	4.31	(18.17)	Gen'd	CH3-CH(CH3)-CH2-CO-CH3
MNBK	Methyl n-Butyl Ketone	100.16	3	-	4	3.55	(16.71)	Gen'd	CH3-CH2-CH2-CH2-CO-CH3
MTBK	Methyl t-Butyl Ketone	100.16	3	-	3	0.78	(8.66)	Gen'd	CH3-C(CH3)(CH3)-CO-CH3
KET6	C6 Ketones	100.16	3	-	8	3.55	(16.71)	L.Mol	MNBK
KET7C	C7 Cyclic Ketones	112.17	4b	-	8	1.41	13.48	L.Mol	CC6-KET
C7-KET-2	2-Heptanone	114.19	2	1	2,4,5	2.80	(15.48)	Gen'd	CH3-CH2-CH2-CH2-CH2-CO-CH3
2M-3-HXO	2-Methyl-3-Hexanone	114.19	3	-	4	1.79	(16.01)	Gen'd	CH3-CH(CH3)-CO-CH2-CH2-CH3
DIPK	Di-Isopropyl Ketone	114.19	3	-	4	1.63	(12.53)	Gen'd	CH3-CH(CH3)-CO-CH(CH3)-CH3
KET7	C7 Ketones	114.19	3	-	8	2.80	(15.48)	L.Mol	C7-KET-2

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
KET8C	C8 Cyclic Ketones	126.20	4b	-	8	1.25	11.99	L.Mol	CC6-KET
C8-KET-2	2-Octanone	128.22	3	-	4	1.66	(13.63)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CO-CH3
KET8	C8 Ketones	128.22	4	-	8	1.66	13.63	L.Mol	C8-KET-2
KET9C	C9 Cyclic Ketones	140.23	4b	-	8	1.13	10.78	L.Mol	CC6-KET
C9-KET-2	2-Nonanone	142.24	3	-	4	1.30	(12.51)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CO-CH3
DIBK	Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	142.24	3	-	4	2.94	(13.42)	Gen'd	CH3-CH(CH3)-CH2-CO-CH2-CH(CH3)-CH3
KET9	C9 Ketones	142.24	4	-	8	1.30	12.51	L.Mol	C9-KET-2
KET10C	C10 Cyclic Ketones	154.25	4b	-	8	1.02	9.80	L.Mol	CC6-KET
C10-K-2	2-Decanone	156.27	3	-	4	1.06	(11.55)	Gen'd	CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CO-CH3
KET10	C10 Ketones	156.27	4	-	8	1.06	11.55	L.Mol	C10-K-2
BIACETYL	Biacetyl	86.09	3	7	14	20.73	(22.30)	Expl	
MVK	Methylvinyl ketone	70.09	1	3	2,5,14	8.73	(27.39)	Gen'd	CH2=CH-CO-CH3
HOACET	Hydroxy Acetone	74.08	3	-	3	3.08	(11.78)	Gen'd	CH3-CO-CH2-OH
MEOACET	Methoxy Acetone	88.11	3	-	3	2.14	(17.48)	Gen'd	CH3-O-CH2-CO-CH3
DIACTALC	Diacetone Alcohol	116.16	3	9	4	0.68	(9.97)	Gen'd	CH3-C(CH3)(OH)-CH2-CO-CH3
PHENOL	Phenol	94.11	4	-	14	1.82	17.72	Expl	
CRESOL	Alkyl Phenols	108.14	3c	6	8	2.34	(15.54)	L.Mol	O-CRESOL
M-CRESOL	m-Cresol	108.14	3c	4a	8	2.34	(15.54)	L.Mol	O-CRESOL
P-CRESOL	p-Cresol	108.14	3c	4	8	2.34	(15.54)	L.Mol	O-CRESOL
O-CRESOL	o-Cresol	108.14	3c	4	2,5,14	2.34	(15.54)	Expl	
NO2-BENZ	Nitrobenzene	123.11	6c	-	8	0.067	0.37	Asn'd	
P-TI	Para Toluene Isocyanate	134.15	2c	1	2,9	0.93	(8.29)	Asn'd	
TDI	Toluene Diisocyanate	174.16	2c	1	2,9	-0.132	(7.17)	Asn'd	
MDI	Methylene Diphenylene Diisocyanate	250.26	3c	-	15	0.79	(5.96)	Asn'd	
DM-AMINE	Dimethyl Amine	45.09	6d	-	16	9.37	14.90	Asn'd	
ET-AMINE	Ethyl Amine	45.09	6d	8	16	7.80	14.80	Asn'd	
TM-AMINE	Trimethyl Amine	59.11	6d	8	16	7.06	17.05	Asn'd	
ME-NITRT	Methyl Nitrite	61.04	-	-	17			-	
ETOH-NH2	Ethanolamine	61.08	6d	-	16	5.97	10.97	Asn'd	
DMAE	Dimethylaminoethanol	89.14	6d	8	16	4.76	13.33	Asn'd	
ETOH2-NH	Diethanol Amine	105.14	6d	-	16	4.05	12.78	Asn'd	
ETOH3-N	Triethanolamine	149.19	6d	-	16	2.76	11.25	Asn'd	
ACRYLNIT	Acrylonitrile	53.06	-					-	
NMP	N-Methyl-2-Pyrrolidone	99.13	2	1	18	2.56	(16.66)	Asn'd	

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
CH3-CL	Methyl Chloride	50.49	6d			0.034	0.055	Asn'd	
CL-ETHE	Vinyl Chloride	62.50	6d			2.92	7.73	Asn'd	
C2-CL	Ethyl Chloride	64.52	6d			0.25	0.77	Asn'd	
CL2-ME	Dichloromethane	84.94	6d			0.066	0.104	Asn'd	
C4-CL	1-Chlorobutane	92.57	-					-	
ME-BR	Methyl Bromide	94.95	6d			0.0169	0.027	Asn'd	
11CL2-C2	1,1-Dichloroethane	98.97	6d			0.101	0.32	Asn'd	
12CL2-C2	1,2-Dichloroethane	99.00	6d			0.098	0.31	Asn'd	
C2-BR	Ethyl Bromide	108.97	6d			0.108	0.34	Asn'd	
12CL2-C3	1,2-Dichloropropane	112.99	-					-	
CHCL3	Chloroform	119.39	6d			0.034	0.054	Asn'd	
C3-BR	n-Propyl Bromide	123.00	6d	1a,d	2,19	0.35	1.59	Asn'd	
111-TCE	1,1,1-Trichloroethane	133.42	6d			0.0036	0.0114	Asn'd	
112CL3C2	1,1,2-Trichloroethane	133.42	6d			0.058	0.181	Asn'd	
C4-BR	n-Butyl Bromide	137.03	6d	1a,d	2,19	0.60	3.57	Asn'd	
3CLME-C8	3-(Chloromethyl)-Heptane	148.68	-					-	
CCL4	Carbon Tetrachloride	153.84	1					L.Mol	INERT
ME-BR2	Methylene Bromide	173.85	-					L.Mol	INERT
11BR2-C2	1,2-Dibromoethane	187.88	6d			0.046	0.146	Asn'd	
11CL2ETH	1,1-Dichloroethene	96.95	-					-	
T-12-DCE	Trans-1,2-Dichloroethene	96.95	6d	-	19	0.81	2.41	Asn'd	
CL2IBUTE	2-(Cl-methyl)-3-Cl-Propene	125.00	6d	2a,d	19	1.13	10.72	Gen'd	CH2=C(CH2-Cl)-CH2-Cl
CL3-ETHE	Trichloroethylene	131.40	6d	1d	2,19	0.60	1.78	Asn'd	
CL4-ETHE	Perchloroethylene	165.85	6d	-	19	0.040	0.126	Asn'd	
CL-BEN	Monochlorobenzene	112.56	6d	-	9	0.36	1.97	Asn'd	
CF3-BEN	Benzotrifluoride	146.11	6d	-	9	0.26	0.93	Asn'd	
CL2-BEN	p-Dichlorobenzene	147.01	6d	-	9	0.20	1.11	Asn'd	
PCBTF	p-Trifluoromethyl-Cl-Benzene	180.56	6d	-	9	0.113	0.40	Asn'd	
CCL3NO2	Chloropicerin	164.38	-	-	20			-	
DMS	Dimethyl Sulfide	62.13	-					-	
DMSO	Dimethyl Sulfoxide	78.13	-	1e	21			-	
SI2OME6	Hexamethyldisiloxane	162.39	-e	1c	22			-	
SI2OMEOH	Hydroxymethyldisiloxane	164.36	-e	1c	22			-	
(SIOME)4	D4 Cyclosiloxane	296.64	-e	1c	22			-	
(SIOME)5	D5 Cyclosiloxane	370.80	-e	1c	22			-	

Table C-1 (continued)

Name	Description	MWt	Unc [a]	Exp [b]	Notes [c]	MIR [d]	UL MIR [e]	Representation in Model [f]	
Mixtures									
ARBROG	Base ROG Mixture	14.44		0	23	3.71		Mix	See Table C-5a
RFA-TLEV	TLEV Exhaust -- RFA	14.04		0	24	4.09		Mix	See Table C-5a
PH2-TLEV	TLEV Exhaust -- Phase 2	14.12		0	24	4.05		Mix	See Table C-5a
LPG-TLEV	TLEV Exhaust -- LPG	14.86		0	24	2.11		Mix	See Table C-5a
CNG-TLEV	TLEV Exhaust -- CNG	15.22		0	24	0.75		Mix	See Table C-5a
E85-TLEV	TLEV Exhaust -- E-85	20.74		0	24	2.70		Mix	See Table C-5a
M85-TLEV	TLEV Exhaust -- M-85	27.45		0	24	1.57		Mix	See Table C-5a
RFA-LEV	Final LEV -- RFA	14.03		0	25	3.64		Mix	See Table C-5a
PH2-LEV	Final LEV -- Phase 2	14.22		0	25	3.55		Mix	See Table C-5a
MS-D	Mineral Spirits "D" (Type II-C)	14.08	3a	1	26	0.79		Mix	See Table C-5b
MS-A	Mineral Spirits "A" (Type I-B, 91% Alkanes)	14.10	3a	1	26	1.27		Mix	See Table C-5b
MS-B	Mineral Spirits "B" (Type II-C)	14.11	3a	1	26	0.78		Mix	See Table C-5b
MS-C	Mineral Spirits "C" (Type II-C)	14.12	3a	1	26	0.78		Mix	See Table C-5b
D95	Exxon Exxol(r) D95 Fluid	14.11	3a	1	27	0.67		Mix	See Table C-5b
ISOPARM	Exxon Isopar(r) M Fluid	14.15	3a	1a	27	0.65		Mix	See Table C-5b
OC6-ACET	Oxo-Hexyl Acetate	18.02	3	-	28	1.03		Mix	See Table C-5c
OC7-ACET	Oxo-Heptyl Acetate	17.58	3	-	28	0.97		Mix	See Table C-5c
OC8-ACET	Oxo-Octyl Acetate	17.23	3	-	28	0.96		Mix	See Table C-5c
OC9-ACET	Oxo-Nonyl Acetate	16.89	3a	-	28	0.85		Mix	See Table C-5c
OC10ACET	Oxo-Decyl Acetate	16.71	3a	1	28	0.83		Mix	See Table C-5c
OC12ACET	Oxo-Dodecyl Acetate	16.30	3a	-	28	0.72		Mix	See Table C-5c
OC13ACET	Oxo-Tridecyl Acetate	16.19	3a	-	28	0.67		Mix	See Table C-5c

[a] Uncertainty codes are given in Table C-2.

[b] Experimental data availability codes are given in Table C-3.

[c] Notes on representation of the detailed model species are given in Table C-4.

[d] Maximum incremental reactivity in units of grams O_3 per gram VOC.

[e] Upper limit maximum incremental reactivity in units of grams O_3 per gram VOC. Parentheses indicate that the MIR is not considered to be sufficiently uncertain that use of upper limit values are appropriate.

Table C-1 (continued)

[f] Representation in the mechanism: "Expl" = explicit in the base mechanism; "Asn'd" = mechanistic parameters assigned; "Gen'd" = mechanistic parameters generated using the mechanism generation system, using the structure shown; "L.Mol" = represented on a mole for mole basis by the model species or mixture shown; "-" = not represented in current version of the mechanism; "Mix" = mixture.

Table C-2 Uncertainty codes used in the listing of detailed model species.

No.	Description
-	No representation of this compound has been developed for this version of the mechanism.
0	Compound believed to be unreactive.
1	Considered to be relatively uncertain, or some uncertainties but reactivity is not expected to change significantly.
2	Uncertain mechanism may change somewhat if refined, but change is expected to be less than a factor of two. If the compound is predicted to inhibit O3, changes are not expected to affect predicted inhibition, but may affect magnitude of inhibition. This code is also used for compounds whose reactivities are expected to be highly sensitive to ambient conditions or to changes in the base mechanism.
3	Uncertain and may change if compound is studied (or studied further) or estimation methods are updated. Change in MIR could be as much as a factor of two. This code is also used for (1) compounds whose reactivities are expected to be sensitive to the representation of the reactive products, whose accuracy is difficult to test experimentally and (2) compounds whose reactivities are expected to be highly sensitive to ambient conditions or to changes in the base mechanism.
4	Uncertain and is expected to change if compound is studied or estimation methods are updated. It is recommended that uncertainty adjustments be employed in regulatory applications.
5	Non-negligible chance of the estimate being incorrect in significant respects. It is recommended that uncertainty adjustments be employed in regulatory applications.
6	Current mechanism is probably incorrect, but biases in atmospheric reactivity predictions are uncertain. It is recommended that uncertainty adjustments be employed in regulatory applications.
a	The reactivity of this compound is expected to be sensitive to ambient conditions and/or changes in the base mechanism.
b	Some uncertainty due to differences in reactivities of compounds represented by this class. Look at differences among compounds in this class for the magnitude of this uncertainty.
c	Parameterized mechanism used, with uncertain portions adjusted to fit chamber data for representative compounds.
d	Highly simplified “Placeholder” mechanism used to represent the approximate range of reactivity of this compound. Mechanism does not represent an estimate of the actual mechanism of the compound.
e	The current version of this mechanism does not represent these compounds, but based on previous studies they are expected to be O_3 inhibitors under all conditions.

Table C-3 Notes on availability of experimental data for evaluating mechanisms for the listed detailed model species.

No.	Description
-	No data available to test ozone predictions for this compound.
1	Tested under MIR and other conditions; well tested.
2	Tested under MIR conditions. There may be limited data for other conditions in some cases.
3	Tested under some conditions, but not MIR reactivity.
4	Tested under some conditions, but data are limited, or are of low quality or precision.
5	This compound has not been studied by itself, but its mechanism has been evaluated using experiments where it is formed as the major reactive product, for which model simulations are highly sensitive to assumed mechanisms for this compound.
6	Experimental data are available for some members of this class or for complex mixtures containing significant amounts of compounds of this class.
7	Chamber data may be available to test mechanisms for this compound, but were not used in this evaluation. Data are believed to be limited, of low precision, not well characterized or difficult to characterize, or highly sensitive to chamber effects.
8	There may be chamber data available to test mechanisms for this compound, but their availability and utility for mechanism evaluation have not been assessed.
9	Attempts to conduct chamber experiments with this compound have been unsuccessful because of experimental difficulties. Probably not possible to study this compound using current methods.
a	Model does not successfully simulate results of all chamber experiments. This may be due to experimental difficulties, though mechanism problems cannot be completely ruled out.
b	Reactivity of this compound may be sensitive to the nature of the light source, but data are available only from blacklight chambers. Effect of changing light source is uncertain and needs to be evaluated.
c.	The current version of the mechanism does not represent this compound or the available data were not used to evaluate how it is currently represented.
d	Although there are chamber data available for this compound and the model performance has been evaluated using them, the current mechanism does not represent halogen chemistry and the predictions of the mechanism may be inaccurate in ambient simulations.
e	Chamber data are available that will be used to develop a mechanism for this compound, which is not represented in the current version of the mechanism.

Table C-4. Notes and comments for the listed detailed model species.

No.	Documentation or Comment
1	Mechanism believed to be fairly well established. See Atkinson (1990, 1994, 1997a) reviews.
2	Evaluation of the mechanism for this compound against chamber data is discussed in this report. See Section V and Appendix B.
3	Mechanism was derived using the mechanism generation system discussed in Section III. Lumped product version of the mechanism used for all simulations.
4	Mechanism was derived using the mechanism generation system discussed in Section III. Adjusted product version of the mechanism used when representing this compound in reactivity or mechanism evaluation simulations, and the lumped product version of the mechanism is used when representing this compound in mixtures. See documentation of product lumping approaches.
5	Adjustments were made to mechanism to improve fits to chamber data.
6	It is uncertain whether the compound(s) used to represent this class is most appropriate for all complex mixtures containing this class.
7	The current mechanism gives reasonably good simulations of incremental reactivity experiments of mineral spirits samples believed to contain significant amounts of these compounds (Carter et al, 1997f). See Section V and Appendix B.
8	The appropriateness of the lumped molecule representation for this class is uncertain.
9	Parameterized mechanism used, with uncertain portions adjusted to fit chamber data for representative compounds. See Section IV.
10	Mixture based roughly on terpenes in estimated North American annual biogenic rates given by Guenther et al (2000).
11	An estimated mechanism was derived as discussed in Section IV.B.2.
12	These are present in relatively large amounts in emissions inventories. The specific compound(s) referred to in these classes are unknown. They are assumed to be similar to the Texanol isomers, though the molecular weights are slightly different.
13	Mixture composition for commercial Texanol samples based on information provided by David Morgott of Eastman Kodak Company (private communication, 1999).
14	The reactions of this compound is represented explicitly in the base mechanism. See Section II.C.
15	Mechanism for this compound estimated by analogy from para toluene isocyanate.
16	Mechanisms for amines have not been developed. A placeholder mechanism used to represent their approximate range of reactivity, given the OH rate constant. See Section IV.B.6
17	The reactions for this compound can be added to the mechanism if needed, but this has not been done for the current version of the mechanism.
18	An estimated mechanism was derived as discussed in Section IV.B.3.

Table C-4 (continued)

No.	Documentation or Comment
19	The current version of the mechanism does not provide for representing reactions of ClO_x or BrO_x species. However, earlier versions of the mechanism that did represent these reactions did not perform well simulating chamber data for most of the halogenated compounds that were studied (Carter et al, 1996d, 1997d). A placeholder mechanism is used to estimate the approximate MIR given the compound's OH rate constant. This mechanism probably overestimates the reactivity of these compounds under low NO_x conditions.
20	The current version of the mechanism does not provide for representing reactions of ClO_x species, and this compound is not currently represented. However, an earlier version of the mechanism that did represent these reactions gave reasonably good fits to the chamber data for this compound (Carter et al, 1997h).
21	An experimental and modeling study of the reactivity of this compound is underway at our laboratories.
22	Volatile silicone compounds are not represented in the current version of the mechanism. They have previously been shown to be ozone inhibitors under all conditions likely to occur in the atmosphere (Carter et al, 1992).
23	The Base ROG mixture is used to represent reactive VOCs from all sources in the atmospheric reactivity calculations, as discussed in Section VII.A.1. It is derived from the "all city average" mixture derived by Jeffries et al (1989) from analysis of air quality data, with minor modifications as discussed by Carter (1994a,b). The compositions of this mixture is given on Table C-5a.
24	These are the "Transitional Low Emissions Vehicle" exhaust mixtures used by the California ARB to calculate reactivity adjustment factors for its Clean Fuels, Low-Emissions Vehicle regulations. Composition obtained from the CARB. The compositions of these mixtures are given on Table C-5a.
25	These are "Low Emissions Vehicle" exhaust mixtures provided by the California ARB. The compositions of these mixtures are given on Table C-5a.
26	These are the mineral spirits samples provided by Safety-Kleen Corporation for environmental chamber reactivity studies (Carter et al, 1997f). Contrary to the earlier version of the mechanism discussed by in that report, the current mechanism performs reasonably well in simulating the chamber results for these samples (see Section V and Appendix B). The assumed compositions of these mixtures are given on Table C-5b.
27	These are commercial solvents produced by Exxon Chemical company. The assumed compositions of these solvents were derived as discussed by Carter et al (2000g), and are given in Table C-5b.
28	These represent commercial solvents produced by Exxon Chemical company, and also similar mixtures consisting of esters of C_{6+} branched alcohols. Their assumed compositions were derived as discussed by Carter et al (2000g), and are given in Table C-5e.
29	This was used in part to derive the mechanism for the ISO-PROD model species, as discussed in the documentation of the base mechanism.
30	This was used in part to derive the mechanism for the PROD2 model species, as discussed in the documentation of the base mechanism.

Table C-4 (continued)

No.	Documentation or Comment
31	This was used in part to derive the mechanism for the RNO3 model species, as discussed in the documentation of the base mechanism.

Table C-5. Compositions of mixtures for which model species have been assigned and reactivities have been estimated.

Table C-5a. Compositions of the ambient reactive organic gas (ROG) surrogate and exhaust mixtures.

Model Name	Mixture Names and Compositions [a]								
	ARBROG	RFA-TLEV	PH2-TLEV	M85-TLEV	LPG-TLEV	CNG-TLEV	E85-TLEV	RFA-LEV	PH2-LEV
ETHANE	1.69e-2	1.86e-2	1.45e-2	2.37e-3	4.00e-2	4.44e-1	1.13e-2	2.42e-2	1.98e-2
PROPANE	1.41e-2	1.05e-3	5.44e-4	1.24e-4	2.21e-1	1.72e-2	8.46e-4	1.08e-3	2.13e-3
N-C4	1.81e-2	1.07e-2	2.79e-3	4.44e-3	2.45e-3	1.62e-3	4.39e-3	1.24e-2	3.86e-3
N-C5	6.13e-3	5.21e-3	2.29e-3	1.41e-3	1.26e-3	5.06e-4	1.90e-3	5.91e-3	2.46e-3
N-C6	1.32e-3	2.98e-3	2.23e-3	6.05e-4	3.97e-4	1.77e-5	7.70e-4	4.12e-3	1.77e-3
N-C7	1.20e-3	1.81e-3	1.18e-3	2.19e-4	2.22e-4	6.07e-5	2.69e-4	1.93e-3	1.42e-3
N-C8	7.40e-4	6.14e-4	5.19e-4	2.40e-5	-	-	1.82e-5	8.72e-4	5.48e-4
N-C9	7.43e-4	1.75e-4	1.32e-4	-	-	-	-	2.73e-4	1.66e-4
N-C10	1.84e-3	5.92e-5	5.95e-5	-	-	-	-	7.89e-5	2.40e-4
N-C11	1.65e-4	6.29e-5	4.52e-5	1.76e-5	-	-	-	1.35e-4	3.64e-5
N-C12	3.26e-4	-	3.31e-5	-	-	-	-	-	-
N-C13	1.47e-5	-	-	-	-	-	-	-	-
2-ME-C3	7.88e-3	1.18e-3	-	9.45e-5	2.81e-3	7.07e-4	2.14e-4	-	-
2-ME-C4	1.52e-2	-	-	-	-	-	-	-	-
BR-C5	-	8.35e-3	-	2.21e-3	2.59e-3	8.23e-4	2.27e-3	-	-
22-DM-C4	4.62e-4	1.12e-3	-	1.59e-4	-	-	1.44e-4	-	-
23-DM-C4	9.55e-4	1.91e-3	-	1.27e-4	1.38e-4	-	-	-	-
2-ME-C5	3.55e-3	-	4.86e-3	-	-	-	-	8.28e-3	5.41e-3
3-ME-C5	2.53e-3	-	2.37e-3	-	-	-	-	4.07e-3	2.66e-3
BR-C6	2.39e-4	7.39e-3	-	1.24e-3	5.17e-4	5.30e-5	4.81e-4	-	-
223TM-C4	-	-	2.82e-5	-	-	-	-	-	-
23-DM-C5	1.12e-3	-	1.32e-3	-	-	-	-	-	4.11e-4
24-DM-C5	6.00e-4	-	7.89e-4	-	-	-	-	1.40e-5	2.41e-4
2-ME-C6	-	-	5.35e-4	-	-	-	-	-	1.13e-4
33-DM-C5	-	-	7.04e-5	-	-	-	-	-	-
3-ME-C6	1.27e-3	-	1.63e-3	-	-	-	-	2.10e-3	2.01e-3
BR-C7	2.09e-3	6.79e-3	5.55e-3	1.15e-3	1.16e-3	2.89e-4	8.90e-4	5.75e-3	9.36e-3
234TM-C5	-	-	1.36e-3	-	-	-	-	7.00e-4	1.41e-3
23-DM-C6	-	-	8.77e-4	-	-	-	-	6.26e-4	9.09e-4
24-DM-C6	-	-	4.57e-4	-	-	-	-	-	1.12e-4
25-DM-C6	-	-	3.21e-4	-	-	-	-	-	7.47e-5
2-ME-C7	-	-	2.84e-4	-	-	-	-	-	3.73e-5
3-ME-C7	-	-	3.83e-4	-	-	-	-	-	6.22e-5
4-ME-C7	-	-	1.11e-4	-	-	-	-	-	-
BR-C8	4.03e-3	7.25e-3	2.36e-3	1.30e-3	2.21e-4	7.99e-5	5.81e-4	3.28e-3	3.01e-3
225TM-C6	-	-	8.25e-4	-	-	-	-	6.12e-4	9.53e-4
24-DM-C7	-	-	5.50e-5	-	-	-	-	-	-
BR-C9	1.71e-3	8.54e-4	8.03e-4	1.71e-4	-	-	1.62e-5	7.11e-4	4.88e-4
BR-C10	1.56e-3	3.95e-5	1.98e-4	3.86e-5	-	-	-	3.94e-5	4.00e-5
BR-C11	1.65e-4	-	-	-	-	-	-	-	-
BR-C12	3.26e-4	-	-	-	-	-	-	-	-
BR-C13	1.47e-5	-	-	-	-	-	-	-	-
CYCC5	7.07e-4	1.80e-4	1.01e-4	3.13e-4	-	-	-	2.00e-5	-
CYCC6	6.84e-4	-	2.01e-4	-	-	-	-	3.17e-4	1.52e-4
CYC-C6	-	5.67e-4	-	-	-	-	1.23e-4	-	-
ME-CYCC5	1.61e-3	1.18e-3	1.02e-3	2.61e-4	4.24e-4	1.81e-5	3.20e-4	1.57e-3	8.11e-4
13DMCYC5	-	-	1.58e-4	-	-	-	-	-	1.45e-5
CYC-C7	1.23e-4	7.15e-5	-	-	-	-	-	-	4.34e-5
ME-CYCC6	6.82e-4	6.58e-4	6.18e-4	2.80e-5	1.51e-5	-	1.48e-4	8.71e-4	4.63e-4
CYC-C8	-	8.38e-4	9.43e-4	7.34e-5	1.32e-5	-	7.39e-5	1.12e-3	5.32e-4
ET-CYCC6	1.79e-4	-	7.55e-5	-	-	-	-	-	-
CYC-C10	-	1.80e-4	-	3.91e-5	2.12e-5	-	2.96e-5	-	-
ETHENE	1.35e-2	4.40e-2	3.08e-2	8.90e-3	3.45e-2	5.59e-3	3.59e-2	2.64e-2	2.76e-2
PROPENE	3.18e-3	1.02e-2	1.45e-2	2.87e-3	1.49e-2	7.23e-4	2.17e-3	8.40e-3	1.14e-2
1-BUTENE	1.15e-3	1.33e-3	1.43e-3	1.47e-4	6.35e-4	1.36e-4	3.70e-4	1.02e-3	9.63e-4
1-PENTEN	8.02e-4	2.80e-4	2.41e-4	-	-	-	-	-	-
3M-1-BUT	3.25e-4	2.00e-5	1.01e-4	-	-	-	-	-	-

Table C-5a (continued)

Model Name	Mixture Names and Compositions [a]								
	ARBROG	RFA-TLEV	PH2-TLEV	M85-TLEV	LPG-TLEV	CNG-TLEV	E85-TLEV	RFA-LEV	PH2-LEV
1-HEXENE	3.34e-4	3.34e-4	5.03e-5	-	-	-	-	-	-
C4-OLE1	1.43e-4	-	-	-	-	-	-	-	-
ISOBUTEN	1.15e-3	3.85e-3	1.15e-2	9.78e-4	7.41e-4	2.44e-4	8.87e-4	2.87e-3	1.00e-2
2M-1-BUT	9.17e-4	2.00e-5	3.02e-4	-	-	-	-	4.00e-5	6.08e-5
C5-OLE1	4.39e-4	-	-	-	-	-	-	-	-
C6-OLE1	2.23e-3	-	3.69e-4	-	-	-	-	5.33e-4	3.89e-4
C7-OLE1	1.19e-3	-	1.44e-5	1.12e-4	-	-	-	1.29e-4	7.24e-5
C8-OLE1	2.39e-4	1.10e-3	8.80e-5	1.96e-4	7.94e-5	4.07e-5	1.85e-4	-	-
C9-OLE1	5.20e-4	3.34e-5	1.68e-4	-	1.18e-5	-	-	8.89e-5	6.76e-5
C10-OLE1	9.55e-5	-	-	-	-	-	-	-	-
C11-OLE1	1.91e-4	-	-	-	-	-	-	-	-
C-2-BUTE	9.07e-4	-	4.28e-4	-	-	-	-	-	1.27e-4
C4-OLE2	1.43e-4	-	-	-	-	-	-	-	-
T-2-BUTE	1.15e-3	1.75e-4	2.26e-4	-	-	-	-	-	7.60e-5
2M-2-BUT	5.16e-4	1.60e-4	4.23e-4	7.83e-5	-	-	-	-	8.11e-5
C5-OLE2	3.17e-3	5.40e-4	4.23e-4	-	-	-	-	1.80e-4	2.03e-5
C6-OLE2	1.00e-3	5.34e-4	8.39e-4	-	-	-	-	8.83e-4	5.41e-4
C7-OLE2	4.37e-4	-	5.75e-5	-	-	-	-	-	-
C8-OLE2	2.15e-4	1.10e-3	1.01e-4	1.96e-4	7.94e-5	4.07e-5	1.85e-4	-	-
C9-OLE2	2.44e-4	3.34e-5	3.35e-5	-	1.18e-5	-	-	8.89e-5	6.76e-5
C10-OLE2	9.55e-5	-	-	-	-	-	-	-	-
C11-OLE2	1.91e-4	-	-	-	-	-	-	-	-
CYC-PNTE	-	4.53e-4	2.49e-4	2.42e-4	1.09e-4	-	-	4.12e-5	2.09e-5
CYC-HEXE	1.75e-4	5.13e-5	6.87e-5	-	-	-	-	-	-
13-BUTDE	6.21e-4	8.82e-4	1.28e-3	2.54e-4	1.37e-4	8.44e-5	2.68e-4	7.52e-4	8.15e-4
ISOPRENE	1.30e-3	1.24e-4	3.94e-4	-	-	-	-	-	6.26e-5
C7-OL2D	1.91e-4	-	-	-	-	-	-	-	-
A-PINENE	5.06e-4	-	-	-	-	-	-	-	-
3-CARENE	1.91e-4	-	-	-	-	-	-	-	-
STYRENE	-	5.66e-4	8.94e-4	1.05e-4	-	-	3.98e-5	7.81e-4	6.83e-4
C9-STYR	4.77e-4	-	-	-	-	-	-	-	-
C10-STYR	3.63e-4	-	-	-	-	-	-	-	-
BENZENE	3.29e-3	1.23e-2	6.52e-3	3.41e-3	7.80e-4	1.95e-5	1.49e-3	1.04e-2	7.88e-3
TOLUENE	9.23e-3	1.53e-2	1.24e-2	4.83e-3	1.37e-3	2.64e-4	1.96e-3	1.10e-2	1.28e-2
C2-BENZ	1.28e-3	3.75e-3	3.48e-3	1.01e-3	1.96e-4	7.17e-5	3.52e-4	3.57e-3	3.23e-3
C9-BEN1	1.59e-4	-	-	-	-	-	-	-	-
I-C3-BEN	1.91e-4	4.79e-4	1.88e-4	2.51e-4	-	-	1.73e-5	1.63e-4	1.42e-4
N-C3-BEN	3.61e-4	-	5.40e-4	-	-	-	-	5.60e-4	4.85e-4
C10-BEN1	1.81e-4	3.66e-5	-	2.05e-5	-	-	-	-	6.36e-5
S-C4-BEN	2.29e-4	-	1.05e-5	-	-	-	-	-	-
C11-BEN1	6.51e-4	-	1.90e-5	-	-	-	-	-	-
C12-BEN1	2.39e-5	-	-	-	-	-	-	-	-
M-XYLENE	2.18e-3	4.97e-3	3.54e-3	1.22e-3	4.76e-4	4.30e-5	6.44e-4	4.47e-3	3.17e-3
O-XYLENE	1.83e-3	3.15e-3	2.62e-3	8.79e-4	1.82e-4	2.87e-5	2.93e-4	3.54e-3	2.41e-3
P-XYLENE	2.18e-3	4.32e-3	3.54e-3	1.22e-3	4.76e-4	4.30e-5	6.44e-4	4.47e-3	3.17e-3
C9-BEN2	2.47e-3	2.80e-3	2.63e-3	7.31e-4	9.89e-5	-	2.93e-4	4.25e-3	2.74e-3
C10-BEN2	1.54e-3	5.75e-5	3.05e-4	4.09e-5	-	-	-	-	-
C11-BEN2	9.55e-5	-	3.81e-5	-	-	-	-	-	-
C12-BEN2	8.75e-5	-	-	-	-	-	-	-	-
123-TMB	7.53e-4	7.01e-5	2.35e-5	-	-	-	-	-	1.18e-5
124-TMB	-	2.22e-3	1.60e-3	5.71e-4	3.71e-5	-	2.59e-4	3.12e-3	1.17e-3
135-TMB	7.21e-4	6.54e-4	7.52e-4	2.28e-4	-	-	1.21e-4	1.21e-3	6.74e-4
C9-BEN3	2.36e-3	-	-	-	-	-	-	-	-
C10-BEN3	1.60e-3	-	1.16e-4	-	-	-	-	-	-
C10-BEN4	4.20e-4	-	6.31e-5	4.50e-4	-	-	-	-	1.06e-5
C11-BEN3	9.55e-5	-	-	-	-	-	-	-	-
C12-BEN3	8.75e-5	-	8.70e-6	-	-	-	-	-	-
INDAN	-	2.38e-5	2.39e-5	-	-	-	-	-	-
NAPHTHAL	-	2.19e-5	5.51e-5	6.42e-5	-	-	-	-	-
ACETYLEN	9.74e-3	1.71e-2	1.63e-2	3.79e-3	1.06e-2	9.35e-4	1.48e-2	1.04e-2	1.16e-2
ME-ACTYL	-	-	1.76e-4	-	-	-	-	-	-
ET-ACTYL	-	-	2.61e-4	-	-	-	-	-	-
MEOH	-	-	-	7.03e-1	-	-	-	-	-

Table C-5a (continued)

Model Name	Mixture Names and Compositions [a]								
	ARBROG	RFA-TLEV	PH2-TLEV	M85-TLEV	LPG-TLEV	CNG-TLEV	E85-TLEV	RFA-LEV	PH2-LEV
ETOH	-	-	-	-	-	-	3.28e-1	-	-
MTBE	-	-	2.03e-3	-	-	-	-	-	4.27e-3
FORMALD	7.92e-3	6.92e-3	7.66e-3	4.81e-2	1.48e-2	1.35e-2	1.25e-2	5.00e-3	9.04e-3
ACETALD	4.77e-3	3.09e-3	1.63e-3	1.31e-3	2.97e-3	1.59e-3	3.62e-2	1.88e-3	1.97e-3
PROPALD	7.00e-4	3.87e-4	2.43e-5	-	1.02e-4	-	2.50e-4	-	-
C4-RCHO	3.10e-4	5.84e-5	-	-	-	-	-	-	1.97e-5
C5-RCHO	1.07e-3	1.63e-5	-	-	-	-	-	-	-
C6-RCHO	7.32e-4	-	-	1.37e-4	-	-	-	-	-
ACROLEIN	-	4.51e-4	2.27e-4	9.79e-5	1.85e-4	-	1.11e-4	-	5.07e-5
CROTALD	-	8.01e-5	-	7.83e-5	-	-	-	-	-
BENZALD	1.64e-4	1.45e-4	2.93e-4	7.76e-5	-	-	-	1.32e-5	1.61e-4
ACETONE	3.09e-3	1.76e-3	1.09e-3	2.46e-3	2.15e-3	8.91e-4	1.86e-3	4.11e-4	7.59e-4
MEK	1.10e-3	1.36e-4	1.96e-5	3.81e-5	-	-	-	-	-

[a] ARBROG is ambient mixture used to represent the base ROG in the reactivity simulations, derived as discussed by Carter (1994a,b). The other mixtures are transitional low emissions vehicle (TLEV) or low emissions vehicle (LEV) compositions provided by the California Air Resources Board (Croes, personal communications, 1990-1991).

Table C-5b. Compositions of mineral spirits and solvent mixtures.

Model Name	Mixture Names and Compositions					
	MS-A [a]	MS-B [a]	MS-C [a]	MS-D [a]	D95 [b]	ISOPARM [b]
N-C8	2.47e-4	-	-	-	-	-
N-C9	2.59e-3	-	-	-	-	-
N-C10	7.04e-3	-	-	-	-	-
N-C11	7.46e-3	-	1.06e-2	1.29e-2	-	9.07e-7
N-C12	2.61e-3	1.22e-3	1.13e-2	7.87e-3	8.06e-4	1.27e-5
N-C13	1.77e-4	1.07e-3	4.04e-4	1.63e-4	6.33e-3	3.41e-5
N-C14	-	1.22e-3	-	-	9.19e-3	7.07e-5
N-C15	-	-	-	-	1.02e-3	2.16e-5
N-C16	-	-	-	-	-	5.01e-6
24-DM-C6	4.93e-5	-	-	-	-	-
2-ME-C7	2.47e-5	-	-	-	-	-
4-ME-C7	2.47e-5	-	-	-	-	-
24-DM-C7	6.04e-4	-	-	-	-	-
2-ME-C8	3.02e-4	-	-	-	-	-
4-ME-C8	3.02e-4	-	-	-	-	-
26DM-C8	3.90e-3	1.73e-4	-	-	-	-
2-ME-C9	1.95e-3	8.67e-5	-	-	-	-
4-ME-C9	1.95e-3	8.67e-5	-	-	-	-
26DM-C9	4.29e-3	1.88e-3	1.07e-3	1.50e-3	-	1.90e-4
3-ME-C10	2.14e-3	9.39e-4	5.37e-4	7.52e-4	-	9.51e-5
4-ME-C10	2.14e-3	9.39e-4	5.37e-4	7.52e-4	-	9.51e-5
36DM-C10	3.42e-3	4.63e-3	5.51e-3	8.72e-3	5.74e-4	2.65e-3
3-ME-C11	1.71e-3	2.31e-3	2.75e-3	4.36e-3	2.87e-4	1.33e-3
5-ME-C11	1.71e-3	2.31e-3	2.75e-3	4.36e-3	2.87e-4	1.33e-3
36DM-C11	8.63e-4	6.77e-3	2.68e-3	2.12e-3	4.51e-3	7.16e-3
3-ME-C12	4.32e-4	3.38e-3	1.34e-3	1.06e-3	2.25e-3	3.58e-3
5-ME-C12	4.32e-4	3.38e-3	1.34e-3	1.06e-3	2.25e-3	3.58e-3
37DM-C12	3.58e-5	2.74e-3	-	-	6.54e-3	1.48e-2
3-ME-C13	1.79e-5	1.37e-3	-	-	3.27e-3	7.42e-3
6-ME-C13	1.79e-5	1.37e-3	-	-	3.27e-3	7.42e-3
37DM-C13	-	4.41e-4	-	-	7.28e-4	4.53e-3
3-ME-C14	-	2.21e-4	-	-	3.64e-4	2.27e-3
6-ME-C14	-	2.21e-4	-	-	3.64e-4	2.27e-3
3-ME-C15	-	-	-	-	-	5.25e-4
48DM-C14	-	-	-	-	-	1.05e-3
7-ME-C15	-	-	-	-	-	5.25e-4
ME-CYCC6	1.86e-5	-	-	-	-	-
ET-CYCC6	5.27e-5	-	-	-	-	-
1E4MCYC6	1.11e-3	-	-	-	-	-
C3-CYCC6	1.11e-3	-	-	-	-	-
14DECYC6	3.46e-3	9.00e-4	-	-	-	-
1M3IPCY6	3.46e-3	9.00e-4	-	-	-	-
C4-CYCC6	3.57e-3	9.27e-4	-	-	-	-
13E5MCC6	5.22e-3	3.32e-3	3.79e-3	4.05e-3	-	2.38e-5
1E2PCYC6	5.22e-3	3.32e-3	3.79e-3	4.05e-3	-	2.38e-5
C5-CYCC6	5.37e-3	3.42e-3	3.90e-3	4.17e-3	-	2.45e-5
135ECYC6	2.73e-3	5.33e-3	8.65e-3	7.56e-3	4.82e-4	3.32e-4
1M4C5CY6	2.73e-3	5.33e-3	8.65e-3	7.56e-3	4.82e-4	3.32e-4
C6-CYCC6	2.82e-3	5.49e-3	8.91e-3	7.79e-3	4.97e-4	3.42e-4
13E5PCC6	3.28e-4	3.67e-3	1.96e-3	1.36e-3	3.79e-3	8.96e-4
1M2C6CC6	3.28e-4	3.67e-3	1.96e-3	1.36e-3	3.79e-3	8.96e-4
C7-CYCC6	3.38e-4	3.78e-3	2.02e-3	1.40e-3	3.91e-3	9.23e-4
13P5ECC6	-	1.20e-3	-	-	5.50e-3	1.86e-3
1M4C7CC6	-	1.20e-3	-	-	5.50e-3	1.86e-3
C8-CYCC6	-	1.23e-3	-	-	5.67e-3	1.91e-3
135PCYC6	-	1.30e-4	-	-	6.12e-4	5.67e-4
1M2C8CC6	-	1.30e-4	-	-	6.12e-4	5.67e-4
C9-CYCC6	-	1.34e-4	-	-	6.31e-4	5.84e-4
13P5BCC6	-	-	-	-	-	1.31e-4
1M4C9CY6	-	-	-	-	-	1.31e-4
C10CYCC6	-	-	-	-	-	1.35e-4
1-OCTENE	2.51e-6	-	-	-	-	-

Table C-5b (continued)

Model Name	Mixture Names and Compositions					
	MS-A [a]	MS-B [a]	MS-C [a]	MS-D [a]	D95 [b]	ISOPARM [b]
1-C9E	9.37e-5	-	-	-	-	-
1-C10E	4.42e-4	-	-	-	-	-
1-C11E	6.65e-4	-	-	-	-	-
1-C12E	3.49e-4	-	-	-	-	-
1-C13E	4.17e-5	-	-	-	-	-
T-4-C9E	2.34e-5	-	-	-	-	-
T-4-C10E	1.10e-4	-	-	-	-	-
T-5-C11E	1.66e-4	-	-	-	-	-
T-5-C12E	8.70e-5	-	-	-	-	-
T-5-C13E	1.08e-5	-	-	-	-	-
TOLUENE	1.88e-4	-	-	-	-	-
I-C3-BEN	2.34e-5	-	-	-	-	-
N-C3-BEN	2.76e-4	-	-	-	-	-
M-XYLENE	5.80e-4	-	-	-	-	-
O-XYLENE	6.41e-4	-	-	-	-	-
P-XYLENE	5.67e-4	-	-	-	-	-
123-TMB	1.27e-3	-	-	-	-	-
124-TMB	1.27e-3	-	-	-	-	-
135-TMB	1.31e-3	-	-	-	-	-
NAPHTHAL	2.14e-4	-	-	-	-	-
INERT	1.67e-3	-	-	-	-	-

[a] See Carter et al (1997f) for a discussion of how these compositions were derived.

[b] See Carter et al (2000g) for a discussion of how these compositions were derived.

Table C-5c. Compositions of iso-acetate solvents.

Model Name	Mixture Names and Compositions [a]						
	OC6-ACET	OC7-ACET	OC8-ACET	OC9-ACET	OC10ACET	OC12ACET	OC13ACET
NC6-ACET	4.62e-2	5.57e-3	-	-	-	-	-
2MC5-ACT	2.37e-2	-	-	-	-	-	-
3MC5-ACT	2.87e-2	5.57e-3	-	-	-	-	-
4MC5-ACT	2.12e-2	-	-	-	-	-	-
23MC4ACT	1.87e-3	-	-	-	-	-	-
2MC6-ACT	-	8.18e-3	-	-	-	-	-
3MC6-ACT	-	1.52e-2	-	-	-	-	-
4MC6-ACT	2.85e-3	2.71e-2	3.81e-3	-	-	-	-
5MC6-ACT	-	8.18e-3	-	-	-	-	-
24MC5ACT	-	1.69e-2	-	-	-	-	-
3EC5-ACT	-	5.08e-3	-	-	-	-	-
NC7-ACET	-	7.33e-3	-	-	-	-	-
34MC6ACT	-	1.19e-2	2.00e-2	3.43e-3	7.76e-4	-	-
35MC6ACT	-	-	1.75e-2	-	-	-	-
3EC6-ACT	-	-	1.35e-2	-	-	-	-
4MC7-ACT	-	-	9.75e-3	-	-	-	-
45MC6ACT	-	-	9.75e-3	-	-	-	-
5MC7-ACT	-	-	8.00e-3	-	-	-	-
3MC7-ACT	-	-	7.00e-3	-	-	-	-
24MC6ACT	-	-	7.00e-3	-	-	-	-
NC8-ACET	-	-	1.50e-3	-	-	-	-
36MC7ACT	-	-	-	5.21e-3	-	-	-
35MC7ACT	-	-	2.31e-3	1.86e-2	3.05e-3	-	-
45MC7ACT	-	-	-	5.21e-3	3.05e-3	-	-
46MC7ACT	-	-	-	5.21e-3	-	-	-
24MC7ACT	-	-	-	1.81e-3	-	-	-
2MC8-ACT	-	-	-	1.81e-3	-	-	-
4MC8-ACT	-	-	-	8.39e-3	-	-	-
5MC8-ACT	-	-	-	8.39e-3	-	-	-
3EC7-ACT	-	-	-	5.21e-3	-	-	-
23MC7ACT	-	-	-	1.36e-3	-	-	-
25MC7ACT	-	-	-	3.40e-3	-	-	-
235M6ACT	-	-	-	3.40e-3	-	-	-
NC9-ACET	-	-	-	4.53e-4	-	-	-
36MC8ACT	-	-	-	5.90e-3	2.48e-2	5.43e-4	2.69e-4
46MC8ACT	-	-	-	5.90e-3	2.48e-2	5.43e-4	2.69e-4
3IPC7ACT	-	-	-	5.90e-3	2.48e-2	5.43e-4	2.69e-4
357M8ACT	-	-	-	-	2.49e-3	3.55e-3	2.52e-4
47MC9ACT	-	-	-	-	-	3.55e-3	2.52e-4
3E6M8ACT	-	-	-	-	-	3.55e-3	2.52e-4
368M9ACT	-	-	-	-	-	1.38e-2	4.96e-3
357M9ACT	-	-	-	-	-	1.38e-2	4.96e-3
2357M8AC	-	-	-	-	-	1.38e-2	4.96e-3
2468M8AC	-	-	-	-	-	5.38e-3	1.56e-2
479M10AC	-	-	-	-	-	5.38e-3	1.56e-2
3E67M9AC	-	-	-	-	-	5.38e-3	1.56e-2
3579M10A	-	-	-	-	-	4.24e-4	1.47e-3
5E368M9A	-	-	-	-	-	4.24e-4	1.47e-3
23568M9A	-	-	-	-	-	4.24e-4	1.47e-3

[a] See Carter et al (2000g) for a discussion of how these compositions were derived.

Table C-6. Summary of calculated incremental and relative reactivities in various scales.

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
ARBROG	Base ROG Mixture	3.71	0.63	17%	3.79	2%	1.46	0.28	19%	0.85	0.25	30%	1.00	2.07	0.25	0.41	41%	1.00	1.62	0.40	0.31	31%
CO	Carbon Monoxide	0.06	0.01	21%	0.06	2%	0.04	0.01	20%	0.03	0.01	25%	0.03	0.07	0.01	0.01	34%	0.02	0.04	0.01	0.01	28%
METHANE	Methane	0.01	0.00	20%	0.01	1%	0.01	0.00	19%	0.01	0.00	25%	0.01	0.01	0.00	0.00	30%	0.01	0.01	0.00	0.00	23%
ETHANE	Ethane	0.31	0.08	26%	0.31	1%	0.20	0.06	29%	0.15	0.05	34%	0.16	0.28	0.05	0.04	28%	0.10	0.15	0.04	0.02	23%
PROPANE	Propane	0.56	0.14	24%	0.56	1%	0.36	0.09	26%	0.26	0.08	31%	0.29	0.51	0.10	0.08	27%	0.19	0.27	0.09	0.04	22%
N-C4	n-Butane	1.33	0.34	25%	1.34	1%	0.83	0.24	29%	0.58	0.20	34%	0.64	1.03	0.22	0.15	24%	0.40	0.56	0.19	0.08	20%
N-C5	n-Pentane	1.54	0.40	26%	1.55	1%	0.95	0.28	29%	0.65	0.23	36%	0.70	0.99	0.25	0.16	22%	0.44	0.59	0.22	0.08	18%
N-C6	n-Hexane	1.45	0.40	28%	1.44	0%	0.93	0.30	32%	0.60	0.24	39%	0.63	0.84	0.21	0.15	24%	0.38	0.56	0.17	0.07	20%
N-C7	n-Heptane	1.28	0.38	29%	1.27	0%	0.82	0.28	35%	0.51	0.23	45%	0.51	0.74	0.07	0.16	30%	0.28	0.46	0.05	0.08	29%
N-C8	n-Octane	1.11	0.35	32%	1.11	0%	0.71	0.27	38%	0.42	0.22	52%	0.40	0.64	-0.13	0.17	43%	0.19	0.38	-0.11	0.10	52%
N-C9	n-Nonane	0.95	0.32	34%	0.95	0%	0.61	0.26	42%	0.34	0.21	60%	0.31	0.56	-0.27	0.19	60%	0.12	0.29	-0.23	0.12	98%
N-C10	n-Decane	0.83	0.30	36%	0.82	-1%	0.54	0.24	44%	0.29	0.19	68%	0.25	0.49	-0.36	0.19	78%	0.06	0.23	-0.30	0.12	193%
N-C11	n-Undecane	0.74	0.28	38%	0.73	-1%	0.48	0.23	48%	0.25	0.19	75%	0.21	0.45	-0.45	0.20	98%	0.03	0.20	-0.36	0.13	-
N-C12	n-Dodecane	0.66	0.26	40%	0.66	1%	0.43	0.21	49%	0.22	0.18	80%	0.18	0.41	-0.42	0.19	106%	0.01	0.18	-0.38	0.13	-
N-C13	n-Tridecane	0.62	0.26	42%	0.61	-1%	0.41	0.20	50%	0.21	0.17	82%	0.17	0.40	-0.48	0.19	115%	-0.01	0.16	-0.38	0.13	-
N-C14	n-Tetradecane	0.58	0.25	43%	0.57	-2%	0.38	0.19	51%	0.20	0.17	83%	0.16	0.38	-0.48	0.18	117%	-0.02	0.15	-0.38	0.13	-
N-C15	n-Pentadecane	0.56	0.25	44%	0.56	0%	0.37	0.19	52%	0.20	0.16	81%	0.16	0.37	-0.43	0.18	114%	-0.02	0.15	-0.40	0.13	-
N-C16	n-C16	0.52	0.24	46%	0.51	-2%	0.35	0.18	52%	0.18	0.15	84%	0.14	0.35	-0.44	0.17	120%	-0.03	0.14	-0.37	0.13	-
N-C17	n-C17	0.49	0.23	46%	0.48	-2%	0.33	0.17	52%	0.17	0.14	84%	0.13	0.33	-0.42	0.16	120%	-0.03	0.13	-0.35	0.12	-
N-C18	n-C18	0.46	0.21	46%	0.45	-2%	0.31	0.16	52%	0.16	0.14	84%	0.13	0.31	-0.39	0.15	120%	-0.03	0.13	-0.33	0.11	-
N-C19	n-C19	0.44	0.20	46%	0.43	-2%	0.29	0.15	52%	0.16	0.13	83%	0.12	0.30	-0.37	0.14	120%	-0.03	0.12	-0.31	0.11	-
N-C20	n-C20	0.42	0.19	46%	0.41	-2%	0.28	0.15	52%	0.15	0.12	84%	0.11	0.28	-0.35	0.14	120%	-0.02	0.11	-0.30	0.10	-
N-C21	n-C21	0.40	0.18	46%	0.39	-2%	0.26	0.14	52%	0.14	0.12	84%	0.11	0.27	-0.34	0.13	120%	-0.02	0.11	-0.29	0.10	-
N-C22	n-C22	0.38	0.18	46%	0.37	-2%	0.25	0.13	52%	0.13	0.11	84%	0.10	0.26	-0.32	0.12	120%	-0.02	0.10	-0.27	0.09	-
2-ME-C3	Isobutane	1.35	0.27	20%	1.36	1%	0.80	0.16	20%	0.57	0.14	25%	0.65	1.22	0.26	0.17	26%	0.48	0.71	0.24	0.10	21%
2-ME-C4	Iso-Pentane	1.68	0.39	23%	1.68	0%	1.02	0.26	26%	0.72	0.22	31%	0.80	1.33	0.30	0.19	23%	0.52	0.74	0.27	0.10	19%
22-DM-C3	Neopentane	0.69	0.14	20%	0.71	1%	0.42	0.08	20%	0.29	0.07	25%	0.34	0.62	0.14	0.09	27%	0.24	0.36	0.13	0.05	21%
BR-C5	Branched C5 Alkanes	1.68	0.39	23%	1.68	0%	1.02	0.26	26%	0.72	0.22	31%	0.80	1.33	0.30	0.19	23%	0.52	0.74	0.27	0.10	19%
22-DM-C4	2,2-Dimethyl Butane	1.33	0.31	23%	1.34	1%	0.80	0.20	25%	0.55	0.17	31%	0.61	0.98	0.24	0.13	21%	0.40	0.53	0.21	0.07	17%
23-DM-C4	2,3-Dimethyl Butane	1.14	0.24	21%	1.15	1%	0.69	0.15	21%	0.48	0.13	27%	0.53	0.92	0.21	0.13	24%	0.40	0.58	0.20	0.08	20%
2-ME-C5	2-Methyl Pentane	1.80	0.44	25%	1.82	1%	1.03	0.30	29%	0.68	0.25	36%	0.74	1.00	0.32	0.15	20%	0.47	0.62	0.28	0.07	15%
3-ME-C5	3-Methylpentane	2.07	0.50	24%	2.10	1%	1.21	0.33	27%	0.83	0.28	34%	0.91	1.37	0.37	0.19	21%	0.58	0.78	0.32	0.10	17%
BR-C6	Branched C6 Alkanes	1.53	0.35	23%	1.55	1%	0.91	0.23	25%	0.62	0.19	31%	0.68	1.04	0.28	0.14	21%	0.46	0.62	0.25	0.08	17%
223TM-C4	2,2,3-Trimethyl Butane	1.32	0.26	20%	1.34	1%	0.76	0.15	19%	0.51	0.13	26%	0.58	0.96	0.26	0.13	22%	0.44	0.61	0.23	0.08	18%
22-DM-C5	2,2-Dimethyl Pentane	1.22	0.29	24%	1.23	1%	0.72	0.20	28%	0.47	0.17	35%	0.52	0.68	0.22	0.10	19%	0.33	0.45	0.19	0.05	15%
23-DM-C5	2,3-Dimethyl Pentane	1.55	0.37	24%	1.57	1%	0.90	0.24	26%	0.60	0.20	33%	0.65	0.89	0.27	0.13	20%	0.43	0.60	0.24	0.07	16%
24-DM-C5	2,4-Dimethyl Pentane	1.65	0.38	23%	1.66	1%	0.94	0.24	26%	0.62	0.21	33%	0.68	0.94	0.31	0.13	19%	0.46	0.60	0.28	0.06	14%
2-ME-C6	2-Methyl Hexane	1.37	0.36	27%	1.38	0%	0.83	0.26	31%	0.52	0.21	40%	0.54	0.74	0.21	0.13	25%	0.33	0.49	0.15	0.07	21%
33-DM-C5	3,3-Dimethyl Pentane	1.32	0.34	26%	1.34	1%	0.80	0.23	28%	0.54	0.19	35%	0.59	0.86	0.23	0.12	21%	0.36	0.49	0.20	0.06	17%
3-ME-C6	3-Methyl Hexane	1.86	0.48	26%	1.87	1%	1.06	0.32	31%	0.69	0.27	39%	0.73	0.99	0.32	0.16	21%	0.44	0.62	0.27	0.08	18%
BR-C7	Branched C7 Alkanes	1.63	0.40	24%	1.64	1%	0.94	0.27	28%	0.61	0.22	36%	0.66	0.86	0.29	0.13	20%	0.42	0.58	0.25	0.07	15%
2233M-C4	2,2,3,3-Tetramethyl Butane	0.44	0.10	22%	0.45	1%	0.27	0.06	23%	0.18	0.05	30%	0.19	0.33	0.08	0.05	23%	0.14	0.19	0.07	0.02	16%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
224TM-C5	2,2,4-Trimethyl Pentane	1.44	0.30	21%	1.45	1%	0.81	0.18	23%	0.54	0.16	29%	0.60	0.91	0.28	0.11	18%	0.43	0.55	0.25	0.06	14%
22-DM-C6	2,2-Dimethyl Hexane	1.13	0.29	25%	1.14	0%	0.67	0.21	31%	0.41	0.17	40%	0.43	0.58	0.17	0.10	23%	0.26	0.39	0.12	0.05	19%
234TM-C5	2,3,4-Trimethyl Pentane	1.23	0.31	25%	1.25	2%	0.72	0.19	27%	0.47	0.16	35%	0.50	0.74	0.21	0.10	21%	0.32	0.47	0.18	0.06	18%
23-DM-C6	2,3-Dimethyl Hexane	1.34	0.34	25%	1.35	1%	0.78	0.23	30%	0.50	0.19	39%	0.52	0.74	0.22	0.12	23%	0.32	0.48	0.16	0.07	21%
24-DM-C6	2,4-Dimethyl Hexane	1.80	0.45	25%	1.83	1%	1.01	0.30	30%	0.63	0.25	39%	0.67	0.89	0.32	0.14	21%	0.40	0.60	0.19	0.08	21%
25-DM-C6	2,5-Dimethyl Hexane	1.68	0.41	24%	1.70	1%	0.93	0.27	29%	0.59	0.22	38%	0.62	0.83	0.28	0.13	22%	0.39	0.58	0.19	0.08	20%
2-ME-C7	2-Methyl Heptane	1.20	0.35	29%	1.20	0%	0.74	0.26	36%	0.44	0.21	49%	0.43	0.65	-0.06	0.16	37%	0.22	0.39	-0.06	0.09	42%
3-ME-C7	3-Methyl Heptane	1.35	0.38	29%	1.36	1%	0.82	0.28	35%	0.50	0.23	47%	0.50	0.73	0.03	0.16	32%	0.26	0.45	-0.01	0.09	35%
4-ME-C7	4-Methyl Heptane	1.48	0.41	28%	1.49	1%	0.86	0.29	34%	0.53	0.24	45%	0.54	0.76	0.12	0.16	29%	0.29	0.47	0.03	0.09	31%
BR-C8	Branched C8 Alkanes	1.57	0.41	26%	1.59	1%	0.90	0.29	32%	0.56	0.24	42%	0.58	0.79	0.18	0.15	26%	0.33	0.51	0.09	0.09	26%
225TM-C6	2,2,5-Trimethyl Hexane	1.33	0.32	24%	1.33	1%	0.73	0.21	29%	0.46	0.18	39%	0.48	0.63	0.23	0.10	21%	0.30	0.43	0.15	0.05	18%
235TM-C6	2,3,5-Trimethyl Hexane	1.33	0.34	26%	1.34	1%	0.79	0.23	29%	0.49	0.19	39%	0.51	0.73	0.20	0.12	24%	0.30	0.47	0.12	0.07	23%
24-DM-C7	2,4-Dimethyl Heptane	1.48	0.40	27%	1.50	1%	0.84	0.28	34%	0.50	0.23	47%	0.50	0.73	0.01	0.16	32%	0.26	0.45	-0.05	0.10	39%
2-ME-C8	2-Methyl Octane	0.96	0.32	33%	0.96	0%	0.60	0.25	41%	0.33	0.20	61%	0.30	0.54	-0.31	0.19	63%	0.11	0.29	-0.25	0.12	105%
33-DE-C5	3,3-Diethyl Pentane	1.35	0.37	27%	1.37	2%	0.79	0.25	31%	0.51	0.20	40%	0.54	0.71	0.22	0.12	21%	0.30	0.44	0.16	0.06	21%
35-DM-C7	3,5-Dimethyl Heptane	1.63	0.44	27%	1.65	1%	0.92	0.31	33%	0.57	0.25	44%	0.58	0.82	0.13	0.17	29%	0.30	0.52	-0.01	0.11	37%
4-ET-C7	4-Ethyl Heptane	1.44	0.41	29%	1.45	0%	0.84	0.30	36%	0.51	0.25	48%	0.51	0.75	0.02	0.17	34%	0.25	0.44	-0.07	0.11	44%
4-ME-C8	4-Methyl Octane	1.08	0.34	32%	1.06	-1%	0.67	0.27	40%	0.38	0.21	56%	0.36	0.59	-0.21	0.18	51%	0.15	0.33	-0.19	0.11	75%
BR-C9	Branched C9 Alkanes	1.25	0.36	29%	1.26	0%	0.74	0.27	37%	0.43	0.22	51%	0.42	0.65	-0.12	0.17	42%	0.20	0.38	-0.13	0.11	55%
24-DM-C8	2,4-Dimethyl Octane	1.09	0.34	31%	1.09	0%	0.65	0.26	41%	0.37	0.21	59%	0.34	0.59	-0.26	0.19	57%	0.13	0.30	-0.25	0.13	98%
26DM-C8	2,6-Dimethyl Octane	1.27	0.37	29%	1.28	1%	0.72	0.27	38%	0.42	0.22	53%	0.41	0.64	-0.14	0.18	45%	0.17	0.37	-0.20	0.13	74%
2-ME-C9	2-Methyl Nonane	0.86	0.31	36%	0.85	0%	0.55	0.25	45%	0.30	0.20	68%	0.26	0.51	-0.36	0.20	78%	0.06	0.25	-0.34	0.13	-
34-DE-C6	3,4-Diethyl Hexane	1.20	0.33	27%	1.19	0%	0.69	0.24	35%	0.42	0.19	46%	0.43	0.61	0.08	0.13	29%	0.22	0.37	0.00	0.08	35%
3-ME-C9	3-Methyl Nonane	0.89	0.31	35%	0.88	-1%	0.56	0.24	44%	0.30	0.20	67%	0.26	0.51	-0.37	0.20	77%	0.07	0.25	-0.33	0.13	187%
4-ME-C9	4-Methyl Nonane	0.99	0.33	34%	0.98	-1%	0.61	0.26	42%	0.34	0.21	63%	0.30	0.55	-0.30	0.20	65%	0.10	0.28	-0.28	0.13	130%
4-PR-C7	4-Propyl Heptane	1.24	0.38	31%	1.25	0%	0.73	0.28	39%	0.42	0.23	55%	0.41	0.65	-0.13	0.19	46%	0.17	0.35	-0.19	0.12	74%
BR-C10	Branched C10 Alkanes	1.09	0.35	32%	1.10	0%	0.65	0.26	40%	0.37	0.21	58%	0.34	0.58	-0.23	0.19	55%	0.12	0.31	-0.25	0.13	103%
26DM-C9	2,6-Dimethyl Nonane	0.95	0.31	33%	0.95	0%	0.56	0.24	43%	0.31	0.20	64%	0.28	0.51	-0.29	0.19	68%	0.08	0.26	-0.30	0.13	162%
35-DE-C7	3,5-Diethyl Heptane	1.21	0.37	31%	1.22	1%	0.69	0.27	39%	0.40	0.23	57%	0.38	0.62	-0.19	0.19	51%	0.12	0.34	-0.30	0.15	124%
3-ME-C10	3-Methyl Decane	0.77	0.29	38%	0.77	1%	0.49	0.23	47%	0.26	0.19	73%	0.22	0.46	-0.42	0.20	92%	0.03	0.21	-0.37	0.13	-
4-ME-C10	4-Methyl Decane	0.80	0.30	37%	0.80	0%	0.51	0.23	46%	0.27	0.19	73%	0.23	0.48	-0.41	0.20	89%	0.04	0.21	-0.36	0.13	-
BR-C11	Branched C11 alkanes	0.87	0.30	35%	0.87	1%	0.53	0.24	45%	0.29	0.19	68%	0.25	0.49	-0.35	0.20	78%	0.06	0.24	-0.33	0.13	-
36-DE-C8	2,6-Diethyl Octane	1.09	0.35	32%	1.11	1%	0.64	0.26	40%	0.38	0.22	58%	0.35	0.59	-0.19	0.19	53%	0.11	0.31	-0.26	0.13	117%
36DM-C10	3,6-Dimethyl Decane	0.88	0.32	36%	0.88	0%	0.54	0.24	45%	0.30	0.20	69%	0.26	0.52	-0.37	0.20	78%	0.05	0.24	-0.36	0.14	-
3-ME-C11	3-Methyl Undecane	0.70	0.28	39%	0.70	0%	0.45	0.22	49%	0.23	0.18	77%	0.19	0.43	-0.42	0.20	104%	0.01	0.19	-0.38	0.14	-
5-ME-C11	5-Methyl Undecane	0.72	0.28	39%	0.71	-2%	0.46	0.22	48%	0.24	0.19	79%	0.19	0.43	-0.45	0.20	107%	0.01	0.18	-0.39	0.14	-
BR-C12	Branched C12 Alkanes	0.80	0.30	37%	0.79	0%	0.50	0.23	46%	0.27	0.19	73%	0.22	0.47	-0.40	0.20	90%	0.03	0.21	-0.37	0.14	-
36DM-C11	3,6-Dimethyl Undecane	0.82	0.30	37%	0.82	0%	0.50	0.23	46%	0.27	0.20	72%	0.24	0.47	-0.39	0.20	83%	0.03	0.21	-0.38	0.14	-
37-DE-C9	3,7-Diethyl Nonane	1.08	0.34	32%	1.08	0%	0.61	0.25	41%	0.35	0.21	60%	0.33	0.56	-0.20	0.18	54%	0.09	0.28	-0.29	0.14	146%
3-ME-C12	3-Methyl Dodecane	0.64	0.26	41%	0.63	-2%	0.41	0.21	50%	0.21	0.17	81%	0.17	0.40	-0.47	0.19	115%	-0.01	0.16	-0.39	0.13	-
5-ME-C12	5-Methyl Dodecane	0.64	0.27	42%	0.64	0%	0.42	0.21	50%	0.21	0.18	83%	0.17	0.41	-0.48	0.20	116%	-0.01	0.16	-0.39	0.14	-
BR-C13	Branched C13 Alkanes	0.73	0.28	39%	0.73	0%	0.46	0.22	48%	0.24	0.19	76%	0.20	0.44	-0.43	0.20	96%	0.01	0.19	-0.39	0.14	-
37DM-C12	3,7-Dimethyl Dodecane	0.74	0.28	38%	0.75	0%	0.46	0.22	48%	0.24	0.18	76%	0.21	0.44	-0.43	0.19	93%	0.01	0.19	-0.37	0.14	-
38DE-C10	3,8-Diethyl Decane	0.68	0.28	41%	0.67	-2%	0.43	0.21	49%	0.23	0.18	76%	0.19	0.42	-0.41	0.19	98%	-0.01	0.18	-0.40	0.14	-
3-ME-C13	3-Methyl Tridecane	0.57	0.25	43%	0.57	0%	0.37	0.20	53%	0.19	0.16	85%	0.15	0.38	-0.42	0.18	123%	-0.02	0.15	-0.39	0.13	-

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
6-ME-C13	6-Methyl Tridecane	0.62	0.26	42%	0.62	0%	0.40	0.20	51%	0.21	0.17	83%	0.16	0.40	-0.48	0.19	119%	-0.01	0.16	-0.40	0.13	-
BR-C14	Branched C14 Alkanes	0.67	0.27	40%	0.67	0%	0.42	0.21	50%	0.22	0.18	79%	0.18	0.41	-0.44	0.19	104%	0.00	0.17	-0.38	0.14	-
37DM-C13	3,7-Dimethyl Tridecane	0.64	0.26	41%	0.65	0%	0.41	0.20	50%	0.21	0.17	80%	0.17	0.40	-0.45	0.19	109%	-0.01	0.16	-0.40	0.14	-
39DE-C11	3,9-Diethyl Undecane	0.62	0.26	42%	0.61	-1%	0.39	0.20	51%	0.21	0.17	82%	0.16	0.39	-0.46	0.18	111%	-0.02	0.15	-0.40	0.14	-
3-ME-C14	3-Methyl Tetradecane	0.53	0.24	44%	0.53	0%	0.35	0.18	52%	0.18	0.15	85%	0.14	0.35	-0.45	0.18	128%	-0.03	0.14	-0.39	0.13	-
6-ME-C14	6-Methyl Tetradecane	0.57	0.25	43%	0.57	-1%	0.38	0.19	51%	0.19	0.16	86%	0.15	0.37	-0.48	0.19	125%	-0.02	0.15	-0.40	0.13	-
BR-C15	Branched C15 Alkanes	0.60	0.25	42%	0.60	0%	0.39	0.20	50%	0.20	0.17	82%	0.16	0.38	-0.46	0.18	117%	-0.02	0.15	-0.40	0.13	-
3-ME-C15	3-Methyl Pentadecane	0.50	0.23	45%	0.50	-1%	0.33	0.18	53%	0.17	0.15	87%	0.13	0.33	-0.48	0.17	133%	-0.03	0.13	-0.39	0.13	-
48DM-C14	4,8-Dimethyl Tetradecane	0.58	0.25	43%	0.57	-2%	0.37	0.19	51%	0.20	0.16	83%	0.16	0.36	-0.44	0.18	112%	-0.02	0.14	-0.39	0.13	-
7-ME-C15	7-Methyl Pentadecane	0.51	0.23	45%	0.51	-2%	0.34	0.18	52%	0.18	0.15	87%	0.13	0.34	-0.43	0.17	130%	-0.03	0.13	-0.40	0.13	-
BR-C16	Branched C16 Alkanes	0.54	0.24	44%	0.53	-2%	0.36	0.18	52%	0.18	0.16	85%	0.14	0.34	-0.45	0.17	121%	-0.03	0.14	-0.39	0.13	-
BR-C17	Branched C17 Alkanes	0.51	0.23	44%	0.50	-2%	0.33	0.17	52%	0.17	0.15	85%	0.14	0.32	-0.42	0.16	121%	-0.03	0.13	-0.37	0.12	-
BR-C18	Branched C18 Alkanes	0.48	0.21	44%	0.48	-2%	0.32	0.16	52%	0.16	0.14	85%	0.13	0.31	-0.40	0.15	121%	-0.03	0.12	-0.35	0.11	-
CYCC3	Cyclopropane	0.10	0.03	27%	0.10	1%	0.07	0.02	32%	0.05	0.02	37%	0.05	0.08	0.02	0.01	27%	0.03	0.05	0.02	0.01	22%
CYCC4	Cyclobutane	1.05	0.30	29%	1.06	1%	0.68	0.23	33%	0.48	0.19	40%	0.52	0.78	0.17	0.14	27%	0.29	0.42	0.15	0.07	24%
CYCC5	Cyclopentane	2.69	0.65	24%	2.72	1%	1.53	0.41	27%	1.03	0.35	34%	1.13	1.60	0.49	0.22	20%	0.74	0.97	0.43	0.12	16%
CYCC6	Cyclohexane	1.46	0.39	26%	1.47	1%	0.90	0.28	31%	0.57	0.23	40%	0.60	0.83	0.23	0.14	24%	0.36	0.54	0.20	0.08	21%
IPR-CC3	Isopropyl Cyclopropane	1.52	0.37	25%	1.53	1%	0.94	0.27	28%	0.66	0.23	34%	0.73	1.12	0.27	0.17	23%	0.45	0.63	0.24	0.08	19%
ME-CYCC5	Methylcyclopentane	2.42	0.58	24%	2.46	1%	1.33	0.38	28%	0.87	0.31	36%	0.94	1.23	0.45	0.17	18%	0.59	0.80	0.39	0.09	16%
CYC-C6	C6 Cycloalkanes	1.46	0.39	26%	1.47	1%	0.90	0.28	31%	0.57	0.23	40%	0.60	0.83	0.23	0.14	24%	0.36	0.54	0.20	0.08	21%
13DMCYC5	1,3-Dimeth. Cyclopentane	2.15	0.52	24%	2.18	2%	1.15	0.34	29%	0.72	0.28	39%	0.77	0.99	0.40	0.15	20%	0.46	0.67	0.20	0.10	21%
CYCC7	Cycloheptane	2.26	0.58	26%	2.30	2%	1.21	0.38	31%	0.78	0.32	41%	0.81	1.11	0.41	0.20	24%	0.46	0.75	0.13	0.14	31%
ET-CYCC5	Ethyl Cyclopentane	2.27	0.58	26%	2.30	1%	1.24	0.38	31%	0.78	0.32	41%	0.83	1.12	0.40	0.18	22%	0.48	0.71	0.19	0.11	24%
ME-CYCC6	Methylcyclohexane	1.99	0.51	26%	2.01	1%	1.11	0.34	31%	0.69	0.28	41%	0.72	0.99	0.25	0.18	25%	0.42	0.66	0.12	0.11	26%
CYC-C7	C7 Cycloalkanes	1.99	0.51	26%	2.01	1%	1.11	0.34	31%	0.69	0.28	41%	0.72	0.99	0.25	0.18	25%	0.42	0.66	0.12	0.11	26%
13DMCYC6	1,3-Dimethyl Cyclohexane	1.72	0.46	27%	1.75	2%	0.94	0.32	34%	0.56	0.27	48%	0.56	0.83	-0.01	0.20	35%	0.29	0.52	-0.10	0.14	48%
CYCC8	Cyclooctane	1.73	0.48	28%	1.75	1%	0.94	0.33	35%	0.57	0.28	49%	0.57	0.86	0.00	0.21	37%	0.26	0.53	-0.17	0.16	61%
ET-CYCC6	Ethylcyclohexane	1.75	0.48	27%	1.77	1%	0.99	0.33	34%	0.60	0.27	45%	0.61	0.88	0.09	0.19	32%	0.32	0.56	-0.03	0.13	40%
PR-CYCC5	Propyl Cyclopentane	1.91	0.51	27%	1.94	1%	1.03	0.35	33%	0.63	0.29	45%	0.65	0.91	0.15	0.18	28%	0.34	0.56	-0.03	0.13	38%
CYC-C8	C8 Cycloalkanes	1.75	0.48	27%	1.77	1%	0.99	0.33	34%	0.60	0.27	45%	0.61	0.88	0.09	0.19	32%	0.32	0.56	-0.03	0.13	40%
BCYC-C9	C9 Bicycloalkanes	1.57	0.45	29%	1.59	1%	0.88	0.32	37%	0.52	0.27	51%	0.51	0.79	-0.09	0.21	41%	0.23	0.46	-0.19	0.15	65%
113MCYC6	1,1,3-Trimethyl Cyclohex.	1.37	0.38	28%	1.38	1%	0.76	0.27	35%	0.44	0.22	51%	0.42	0.66	-0.17	0.18	44%	0.20	0.39	-0.18	0.13	63%
1E4MCYC6	1-Eth.-4-Meth. Cyclohex.	1.62	0.46	28%	1.64	1%	0.89	0.32	36%	0.53	0.27	51%	0.52	0.81	-0.06	0.21	40%	0.23	0.47	-0.20	0.15	67%
C3-CYCC6	Propyl Cyclohexane	1.47	0.43	29%	1.49	1%	0.84	0.31	37%	0.49	0.25	52%	0.48	0.75	-0.12	0.20	42%	0.22	0.43	-0.18	0.14	64%
CYC-C9	C9 Cycloalkanes	1.55	0.44	29%	1.57	1%	0.86	0.32	37%	0.51	0.26	51%	0.50	0.78	-0.09	0.21	41%	0.22	0.45	-0.19	0.15	65%
BCYC-C10	C10 Bicycloalkanes	1.29	0.40	31%	1.29	0%	0.74	0.29	39%	0.43	0.24	56%	0.40	0.67	-0.20	0.21	52%	0.15	0.38	-0.28	0.15	102%
13DECYC6	1,3-Diethyl-Cyclohexane	1.34	0.41	30%	1.36	1%	0.75	0.29	39%	0.43	0.24	57%	0.41	0.69	-0.23	0.22	53%	0.13	0.38	-0.32	0.16	122%
14DECYC6	1,4-Diethyl-Cyclohexane	1.49	0.44	30%	1.49	0%	0.82	0.31	38%	0.48	0.26	53%	0.47	0.74	-0.12	0.21	45%	0.18	0.43	-0.26	0.16	89%
1M3IPCY6	1-Meth.-3-Isopr. Cyclohex.	1.26	0.38	30%	1.26	0%	0.72	0.27	37%	0.42	0.22	53%	0.40	0.66	-0.16	0.19	48%	0.16	0.39	-0.22	0.14	84%
C4-CYCC6	Butyl Cyclohexane	1.07	0.36	33%	1.07	0%	0.64	0.27	43%	0.36	0.23	63%	0.32	0.59	-0.35	0.22	68%	0.09	0.30	-0.33	0.15	158%
CYC-C10	C10 Cycloalkanes	1.27	0.39	31%	1.27	0%	0.73	0.28	39%	0.42	0.24	56%	0.40	0.66	-0.20	0.21	52%	0.15	0.37	-0.27	0.15	102%
BCYC-C11	C11 Bicycloalkanes	1.01	0.35	35%	1.01	0%	0.59	0.26	44%	0.32	0.22	68%	0.28	0.55	-0.44	0.22	79%	0.04	0.26	-0.42	0.17	-
13E5MCC6	13-Dieth-5-Me. Cyclohex.	1.11	0.37	33%	1.11	0%	0.62	0.27	43%	0.34	0.22	66%	0.31	0.58	-0.42	0.22	72%	0.05	0.28	-0.43	0.18	-
1E2PCYC6	1-Ethyl-2-Propyl Cyclohex.	0.95	0.35	36%	0.95	0%	0.58	0.26	45%	0.32	0.22	69%	0.27	0.55	-0.48	0.23	84%	0.03	0.26	-0.44	0.17	-
C5-CYCC6	Pentyl Cyclohexane	0.91	0.32	36%	0.91	0%	0.55	0.25	45%	0.30	0.21	70%	0.26	0.52	-0.41	0.21	83%	0.04	0.24	-0.39	0.15	-

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
CYC-C11	C11 Cycloalkanes	0.99	0.35	35%	0.99	0%	0.58	0.26	44%	0.32	0.22	68%	0.28	0.55	-0.44	0.22	79%	0.04	0.26	-0.42	0.17	-
CYC-C11	C11 Cycloalkanes	0.99	0.35	35%	0.99	0%	0.58	0.26	44%	0.32	0.22	68%	0.28	0.55	-0.44	0.22	79%	0.04	0.26	-0.42	0.17	-
BCYC-C12	C12 Bicycloalkanes	0.88	0.32	37%	0.89	1%	0.52	0.24	46%	0.28	0.20	71%	0.24	0.50	-0.43	0.21	86%	0.02	0.22	-0.43	0.16	-
CYC-C12	C12 Cycloalkanes	0.87	0.32	37%	0.88	1%	0.52	0.24	46%	0.28	0.20	71%	0.24	0.50	-0.43	0.21	86%	0.02	0.22	-0.42	0.16	-
135ECYC6	1,3,5-Triethyl Cyclohex.	1.06	0.36	34%	1.07	1%	0.60	0.26	44%	0.33	0.22	67%	0.30	0.57	-0.42	0.22	74%	0.03	0.26	-0.45	0.18	-
1M4C5CY6	1-Meth.-4-Pentyl Cyclohex.	0.81	0.31	39%	0.83	3%	0.49	0.22	46%	0.27	0.19	70%	0.23	0.46	-0.37	0.19	82%	0.02	0.21	-0.37	0.14	-
C6-CYCC6	Hexyl Cyclohexane	0.75	0.30	39%	0.75	0%	0.47	0.23	49%	0.25	0.19	79%	0.20	0.45	-0.51	0.21	107%	0.00	0.19	-0.44	0.15	-
BCYC-C13	C13 Bicycloalkanes	0.79	0.31	39%	0.80	1%	0.48	0.23	48%	0.26	0.20	78%	0.21	0.46	-0.50	0.21	100%	-0.01	0.20	-0.45	0.16	-
13E5PCC6	13-Dieth-5-Pent Cyclohx.	0.99	0.35	35%	1.01	1%	0.56	0.25	45%	0.31	0.21	68%	0.28	0.54	-0.45	0.22	78%	0.02	0.25	-0.46	0.17	-
1M2C6CC6	1-Meth.-2-Hexyl-Cyclohex.	0.70	0.29	42%	0.70	0%	0.44	0.22	51%	0.23	0.19	82%	0.18	0.44	-0.51	0.21	114%	-0.03	0.19	-0.46	0.16	-
C7-CYCC6	Heptyl Cyclohexane	0.66	0.27	42%	0.66	-1%	0.42	0.21	51%	0.22	0.19	86%	0.17	0.42	-0.52	0.21	119%	-0.02	0.17	-0.44	0.15	-
CYC-C13	C13 Cycloalkanes	0.78	0.30	39%	0.79	1%	0.48	0.23	48%	0.25	0.20	78%	0.21	0.46	-0.49	0.21	100%	-0.01	0.20	-0.45	0.16	-
BCYC-C14	C14 Bicycloalkanes	0.71	0.28	40%	0.72	1%	0.44	0.21	49%	0.24	0.18	77%	0.19	0.43	-0.47	0.20	100%	-0.02	0.18	-0.43	0.15	-
13P5ECC6	13-Diprop-5-Eth Cyclohx.	0.94	0.33	35%	0.94	0%	0.53	0.24	46%	0.30	0.20	69%	0.26	0.51	-0.43	0.20	78%	0.01	0.23	-0.45	0.17	-
1M4C7CC6	1-Meth.-4-Heptyl Cyclohex.	0.58	0.27	46%	0.60	4%	0.38	0.19	51%	0.20	0.16	80%	0.16	0.37	-0.42	0.18	109%	-0.03	0.15	-0.40	0.14	-
C8-CYCC6	Octyl Cyclohexane	0.60	0.26	44%	0.60	0%	0.39	0.20	52%	0.20	0.18	87%	0.16	0.39	-0.53	0.20	128%	-0.03	0.15	-0.44	0.15	-
CYC-C14	C14 Cycloalkanes	0.71	0.28	40%	0.71	1%	0.43	0.21	49%	0.23	0.18	77%	0.19	0.42	-0.46	0.19	100%	-0.02	0.18	-0.43	0.15	-
BCYC-C15	C15 Bicycloalkanes	0.69	0.28	41%	0.69	0%	0.42	0.21	50%	0.23	0.18	78%	0.19	0.41	-0.45	0.19	101%	-0.02	0.17	-0.42	0.15	-
135PCYC6	135-Tripropyl Cyclohex.	0.90	0.32	35%	0.90	0%	0.51	0.23	46%	0.29	0.20	69%	0.25	0.50	-0.37	0.19	75%	0.01	0.21	-0.42	0.16	-
1M2C8CC6	1-Methyl-2-Octyl Cyclohex.	0.60	0.27	44%	0.60	-1%	0.39	0.20	51%	0.21	0.17	80%	0.16	0.38	-0.47	0.18	112%	-0.03	0.15	-0.42	0.14	-
C9-CYCC6	Nonyl Cyclohexane	0.54	0.26	47%	0.54	1%	0.36	0.19	54%	0.18	0.16	90%	0.14	0.37	-0.48	0.19	137%	-0.04	0.13	-0.43	0.14	-
CYC-C15	C15 Cycloalkanes	0.68	0.28	41%	0.68	0%	0.42	0.21	50%	0.23	0.18	78%	0.18	0.41	-0.44	0.19	101%	-0.02	0.16	-0.42	0.15	-
13P5BCC6	1,3-Prop.-5-Butyl Cyclohex.	0.77	0.29	38%	0.77	0%	0.45	0.22	48%	0.25	0.18	74%	0.21	0.44	-0.44	0.19	90%	-0.01	0.19	-0.45	0.15	-
1M4C9CY6	1-Methyl-4-Nonyl Cyclohex.	0.55	0.26	47%	0.55	-1%	0.35	0.19	55%	0.19	0.17	88%	0.14	0.36	-0.48	0.18	129%	-0.05	0.13	-0.44	0.14	-
C10CYCC6	Decyl Cyclohexane	0.50	0.24	48%	0.51	1%	0.33	0.18	54%	0.17	0.16	90%	0.13	0.34	-0.48	0.18	136%	-0.05	0.14	-0.42	0.14	-
CYC-C16	C16 Cycloalkanes	0.61	0.26	43%	0.61	0%	0.38	0.20	52%	0.20	0.17	83%	0.16	0.38	-0.47	0.18	114%	-0.04	0.15	-0.43	0.15	-
ETHENE	Ethene	9.08	1.39	15%	9.28	2%	3.70	0.52	14%	2.34	0.52	22%	2.85	4.86	2.43	0.49	17%	2.73	3.74	2.35	0.33	12%
PROPENE	Propene	11.58	1.74	15%	11.91	3%	4.43	0.67	15%	2.83	0.65	23%	3.46	5.83	2.93	0.52	15%	3.41	4.32	3.16	0.26	8%
1-BUTENE	1-Butene	10.29	1.71	17%	10.54	2%	4.03	0.76	19%	2.60	0.69	27%	3.12	4.85	2.65	0.42	14%	2.85	3.30	2.65	0.18	6%
C4-OLE1	C4 Terminal Alkenes	10.29	1.71	17%	10.54	2%	4.03	0.76	19%	2.60	0.69	27%	3.12	4.85	2.65	0.42	14%	2.85	3.30	2.65	0.18	6%
1-PENTEN	1-Pentene	7.79	1.34	17%	7.97	2%	3.11	0.61	20%	2.00	0.55	28%	2.38	3.58	2.01	0.31	13%	2.09	2.41	1.95	0.12	6%
3M-1-BUT	3-Methyl-1-Butene	6.99	1.17	17%	7.19	3%	2.83	0.54	19%	1.85	0.50	27%	2.21	3.44	1.82	0.32	14%	1.97	2.34	1.82	0.13	7%
C5-OLE1	C5 Terminal Alkenes	7.79	1.34	17%	7.97	2%	3.11	0.61	20%	2.00	0.55	28%	2.38	3.58	2.01	0.31	13%	2.09	2.41	1.95	0.12	6%
1-HEXENE	1-Hexene	6.17	1.08	18%	6.33	3%	2.58	0.53	21%	1.69	0.48	28%	1.98	2.93	1.63	0.27	14%	1.70	2.10	1.54	0.12	7%
33M1-BUT	3,3-Dimethyl-1-Butene	6.06	1.01	17%	6.23	3%	2.51	0.45	18%	1.64	0.42	26%	1.95	3.06	1.61	0.28	14%	1.75	2.25	1.58	0.15	8%
3M1-C5E	3-Methyl-1-Pentene	6.22	1.08	17%	6.37	2%	2.54	0.51	20%	1.64	0.46	28%	1.93	2.81	1.61	0.24	12%	1.64	1.91	1.47	0.09	6%
4M1-C5E	4-Methyl-1-Pentene	6.26	1.05	17%	6.43	3%	2.51	0.49	20%	1.61	0.44	28%	1.91	2.81	1.61	0.24	12%	1.65	1.92	1.48	0.09	5%
C6-OLE1	C6 Terminal Alkenes	6.17	1.08	18%	6.33	3%	2.58	0.53	21%	1.69	0.48	28%	1.98	2.93	1.63	0.27	14%	1.70	2.10	1.54	0.12	7%
1-HEPTEN	1-Heptene	4.56	0.85	19%	4.69	3%	1.95	0.45	23%	1.25	0.40	32%	1.43	1.80	1.16	0.17	12%	1.13	1.34	0.79	0.10	9%
1-OCTENE	1-Octene	3.45	0.67	19%	3.53	2%	1.50	0.38	25%	0.94	0.33	35%	1.06	1.37	0.84	0.14	13%	0.77	0.94	0.43	0.11	14%
C8-OLE1	C8 Terminal Alkenes	3.45	0.67	19%	3.53	2%	1.50	0.38	25%	0.94	0.33	35%	1.06	1.37	0.84	0.14	13%	0.77	0.94	0.43	0.11	14%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
1-C9E	1-Nonene	2.76	0.56	20%	2.83	2%	1.22	0.33	27%	0.75	0.29	38%	0.83	1.07	0.56	0.14	17%	0.55	0.75	0.20	0.13	23%
C9-OLE1	C9 Terminal Alkenes	2.76	0.56	20%	2.83	2%	1.22	0.33	27%	0.75	0.29	38%	0.83	1.07	0.56	0.14	17%	0.55	0.75	0.20	0.13	23%
1-C10E	1-Decene	2.28	0.49	21%	2.33	2%	1.02	0.30	29%	0.61	0.25	41%	0.66	0.88	0.33	0.14	21%	0.41	0.60	0.05	0.13	32%
C10-OLE1	C10 Terminal Alkenes	2.28	0.49	21%	2.33	2%	1.02	0.30	29%	0.61	0.25	41%	0.66	0.88	0.33	0.14	21%	0.41	0.60	0.05	0.13	32%
1-C11E	1-Undecene	1.95	0.42	22%	1.97	1%	0.87	0.27	31%	0.52	0.23	44%	0.55	0.77	0.20	0.14	25%	0.32	0.49	-0.04	0.13	42%
C11-OLE1	C11 Terminal Alkenes	1.95	0.42	22%	1.97	1%	0.87	0.27	31%	0.52	0.23	44%	0.55	0.77	0.20	0.14	25%	0.32	0.49	-0.04	0.13	42%
C12-OLE1	C12 Terminal Alkenes	1.72	0.38	22%	1.75	2%	0.77	0.24	31%	0.46	0.21	45%	0.48	0.69	0.10	0.14	29%	0.26	0.43	-0.10	0.13	51%
1-C12E	1-Dodecene	1.72	0.38	22%	1.75	2%	0.77	0.24	31%	0.46	0.21	45%	0.48	0.69	0.10	0.14	29%	0.26	0.43	-0.10	0.13	51%
1-C13E	1-Tridecene	1.55	0.35	23%	1.59	3%	0.69	0.22	32%	0.41	0.19	47%	0.42	0.61	0.03	0.14	32%	0.22	0.38	-0.13	0.13	58%
C13-OLE1	C13 Terminal Alkenes	1.55	0.35	23%	1.59	3%	0.69	0.22	32%	0.41	0.19	47%	0.42	0.61	0.03	0.14	32%	0.22	0.38	-0.13	0.13	58%
1-C14E	1-Tetradecene	1.48	0.33	22%	1.50	1%	0.66	0.20	31%	0.40	0.17	43%	0.43	0.59	0.18	0.10	24%	0.23	0.36	-0.06	0.10	44%
C14-OLE1	C14 Terminal Alkenes	1.48	0.33	22%	1.50	1%	0.66	0.20	31%	0.40	0.17	43%	0.43	0.59	0.18	0.10	24%	0.23	0.36	-0.06	0.10	44%
1-C15E	1-Pentadecene	1.30	0.30	23%	1.31	1%	0.59	0.19	33%	0.34	0.17	49%	0.35	0.52	-0.06	0.13	36%	0.17	0.31	-0.16	0.12	70%
C15-OLE1	C15 Terminal Alkenes	1.30	0.30	23%	1.31	1%	0.59	0.19	33%	0.34	0.17	49%	0.35	0.52	-0.06	0.13	36%	0.17	0.31	-0.16	0.12	70%
ISOBUTEN	Isobutene	6.35	0.75	12%	6.57	3%	2.19	0.27	13%	1.26	0.28	23%	1.56	2.18	1.22	0.23	15%	2.03	2.51	1.66	0.19	9%
2M-1-BUT	2-Methyl-1-Butene	6.51	0.83	13%	6.71	3%	2.35	0.34	15%	1.39	0.33	24%	1.70	2.39	1.42	0.19	11%	2.08	2.56	1.77	0.16	8%
23M1-BUT	23-Dimethyl-1-Butene	4.77	0.63	13%	4.93	3%	1.76	0.27	15%	1.03	0.26	25%	1.25	1.58	1.08	0.11	8%	1.48	1.77	1.25	0.11	7%
2E1-BUT	2-Ethyl-1-Butene	5.04	0.67	13%	5.20	3%	1.85	0.29	16%	1.10	0.27	25%	1.33	1.77	1.16	0.12	9%	1.54	1.82	1.31	0.11	7%
2M1-C5E	2-Methyl-1-Pentene	5.18	0.68	13%	5.34	3%	1.88	0.30	16%	1.11	0.28	25%	1.34	1.73	1.17	0.13	9%	1.59	1.88	1.34	0.12	7%
233M1BUT	2,3,3-trimethyl-1-Butene	4.62	0.69	15%	4.76	3%	1.83	0.31	17%	1.14	0.30	26%	1.35	1.71	1.19	0.12	9%	1.49	1.92	1.22	0.15	10%
C7-OLE1	C7 Terminal Alkenes	4.56	0.85	19%	4.69	3%	1.95	0.45	23%	1.25	0.40	32%	1.43	1.80	1.16	0.17	12%	1.13	1.34	0.79	0.10	9%
3M2I1C4E	3-Methyl-2-Isopropyl-1-Butene	3.29	0.59	18%	3.35	2%	1.42	0.33	23%	0.87	0.29	33%	0.98	1.19	0.81	0.09	10%	0.85	0.99	0.54	0.09	10%
C-2-BUTE	cis-2-Butene	13.22	1.83	14%	13.79	4%	4.75	0.67	14%	2.95	0.67	23%	3.66	6.26	3.07	0.55	15%	4.27	5.31	3.73	0.29	7%
T-2-BUTE	trans-2-Butene	13.91	1.90	14%	14.51	4%	4.89	0.66	14%	2.98	0.66	22%	3.72	6.29	3.04	0.56	15%	4.63	5.82	4.02	0.33	7%
C4-OLE2	C4 Internal Alkenes	13.57	1.87	14%	14.13	4%	4.82	0.67	14%	2.97	0.67	22%	3.69	6.27	3.06	0.55	15%	4.45	5.56	3.87	0.31	7%
2M-2-BUT	2-Methyl-2-Butene	14.45	1.86	13%	15.26	6%	4.65	0.58	13%	2.63	0.62	23%	3.35	5.23	2.23	0.68	20%	5.31	6.98	4.16	0.59	11%
C-2-PENT	cis-2-Pentene	10.24	1.68	16%	10.61	4%	3.87	0.68	18%	2.49	0.65	26%	3.03	5.02	2.58	0.44	15%	2.94	3.28	2.58	0.17	6%
T-2-PENT	trans-2-Pentene	10.23	1.68	16%	10.61	4%	3.87	0.69	18%	2.50	0.65	26%	3.03	5.04	2.58	0.45	15%	2.94	3.27	2.57	0.17	6%
2-C5-OLE	2-Pentenes	10.23	1.68	16%	10.61	4%	3.87	0.69	18%	2.50	0.65	26%	3.03	5.04	2.58	0.45	15%	2.94	3.27	2.58	0.17	6%
C5-OLE2	C5 Internal Alkenes	10.23	1.68	16%	10.61	4%	3.87	0.69	18%	2.50	0.65	26%	3.03	5.04	2.58	0.45	15%	2.94	3.27	2.58	0.17	6%
23M2-BUT	2,3-Dimethyl-2-Butene	13.32	1.89	14%	14.06	6%	3.97	0.51	13%	2.06	0.56	27%	2.69	4.77	1.36	0.86	32%	5.28	7.46	3.58	0.86	16%
2M-2-C5E	2-Methyl-2-Pentene	12.28	1.67	14%	12.87	5%	4.18	0.62	15%	2.37	0.59	25%	2.97	4.27	2.27	0.44	15%	4.29	5.13	3.39	0.42	10%
C-2-C6E	Cis-2-Hexene	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
C-3-C6E	Cis-3-Hexene	8.22	1.52	18%	8.45	3%	3.21	0.68	21%	2.10	0.62	29%	2.52	4.07	2.01	0.42	17%	2.10	2.49	1.65	0.19	9%
C3M2-C5E	Cis-3-Methyl-2-Hexene	13.38	1.81	14%	14.00	5%	4.60	0.66	14%	2.63	0.64	24%	3.29	4.92	2.40	0.54	16%	4.90	6.18	3.87	0.50	10%
T3M2-C5E	Trans 3-Methyl-2-Hexene	14.17	1.92	14%	14.85	5%	4.84	0.68	14%	2.75	0.67	24%	3.45	5.17	2.46	0.60	17%	5.27	6.77	4.15	0.54	10%
T4M2-C5E	Trans 4-Methyl-2-Hexene	7.88	1.25	16%	8.14	3%	3.03	0.54	18%	1.95	0.51	26%	2.36	3.91	2.03	0.34	15%	2.29	2.53	1.94	0.14	6%
T-2-C6E	Trans-2-Hexene	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
T-3-C6E	Trans-3-Hexene	8.16	1.50	18%	8.38	3%	3.18	0.67	21%	2.07	0.61	29%	2.48	4.04	1.99	0.41	17%	2.09	2.47	1.66	0.18	9%
2-C6-OLE	2-Hexenes	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
C6-OLE2	C6 Internal Alkenes	8.44	1.38	16%	8.73	3%	3.23	0.60	19%	2.06	0.55	27%	2.51	4.06	2.15	0.35	14%	2.38	2.62	1.97	0.14	6%
23M2-C5E	2,3-Dimethyl-2-Hexene	10.41	1.43	14%	10.98	5%	3.27	0.41	12%	1.75	0.44	25%	2.24	3.47	1.39	0.54	24%	3.91	5.18	2.86	0.52	13%
C-3-C7E	Cis-3-Heptene	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
T44M2C5E	Trans 4,4-dimethyl-2-Pentene	6.99	1.09	16%	7.22	3%	2.63	0.46	17%	1.65	0.43	26%	2.01	3.12	1.75	0.24	12%	2.03	2.20	1.76	0.10	5%
T-2-C7E	Trans-2-Heptene	7.33	1.22	17%	7.56	3%	2.89	0.56	19%	1.85	0.51	27%	2.22	3.51	1.87	0.31	14%	2.01	2.23	1.53	0.14	7%
T-3-C7E	Trans-3-Heptene	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%
2-C7-OLE	2-Heptenes	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%
C7-OLE2	C7 Internal Alkenes	6.96	1.31	19%	7.15	3%	2.76	0.62	22%	1.81	0.56	31%	2.16	3.40	1.67	0.36	17%	1.71	2.02	1.21	0.18	10%
C-4-C8E	Cis-4-Octene	5.94	1.15	19%	6.09	2%	2.38	0.56	23%	1.57	0.49	31%	1.85	2.80	1.40	0.31	17%	1.39	1.66	0.86	0.17	12%
T22M3C6E	Trans 2,2-Dimethyl 3-Hexene	5.97	1.06	18%	6.16	3%	2.37	0.50	21%	1.54	0.45	29%	1.83	2.67	1.49	0.26	14%	1.53	1.82	1.13	0.13	8%
T25M3C6E	Trans 2,5-Dimethyl 3-Hexene	5.44	1.04	19%	5.58	3%	2.27	0.53	23%	1.53	0.48	31%	1.80	2.77	1.35	0.33	18%	1.33	1.61	0.81	0.17	13%
T-3-C8E	Trans-3-Octene	6.13	1.17	19%	6.30	3%	2.50	0.57	23%	1.64	0.51	31%	1.94	2.99	1.47	0.33	17%	1.46	1.73	0.91	0.17	12%
T-4-C8E	Trans-4-Octene	5.90	1.13	19%	6.09	3%	2.34	0.54	23%	1.53	0.48	31%	1.82	2.80	1.39	0.30	17%	1.39	1.68	0.89	0.17	12%
3-C8-OLE	3-Octenes	6.13	1.17	19%	6.30	3%	2.50	0.57	23%	1.64	0.51	31%	1.94	2.99	1.47	0.33	17%	1.46	1.73	0.91	0.17	12%
C8-OLE2	C8 Internal Alkenes	5.90	1.13	19%	6.09	3%	2.34	0.54	23%	1.53	0.48	31%	1.82	2.80	1.39	0.30	17%	1.39	1.68	0.89	0.17	12%
244M2C5E	2,4,4-trimethyl-2-Pentene	5.85	0.88	15%	6.11	5%	2.08	0.38	18%	1.21	0.33	28%	1.47	1.86	1.21	0.14	10%	1.76	2.16	1.15	0.23	13%
3-C9-OLE	3-Nonenes	5.31	1.03	19%	5.48	3%	2.17	0.52	24%	1.43	0.46	32%	1.68	2.49	1.24	0.28	17%	1.21	1.46	0.66	0.17	14%
C9-OLE2	C9 Internal Alkenes	5.31	1.03	19%	5.48	3%	2.17	0.52	24%	1.43	0.46	32%	1.68	2.49	1.24	0.28	17%	1.21	1.46	0.66	0.17	14%
T-4-C9E	Trans-4-Nonene	5.23	1.01	19%	5.39	3%	2.14	0.51	24%	1.40	0.45	32%	1.65	2.45	1.22	0.28	17%	1.19	1.43	0.65	0.17	14%
34E2-C6E	3,4-Diethyl-2-Hexene	3.95	0.87	22%	4.04	2%	1.81	0.52	29%	1.14	0.45	39%	1.27	1.73	0.83	0.22	17%	0.82	1.16	0.10	0.22	27%
C-5-C10E	Cis-5-Decene	4.89	0.95	20%	5.03	3%	2.04	0.50	24%	1.35	0.44	32%	1.57	2.32	1.15	0.27	17%	1.10	1.33	0.54	0.17	15%
T-4-C10E	Trans-4-Decene	4.50	0.89	20%	4.62	3%	1.86	0.46	25%	1.21	0.40	33%	1.42	2.08	1.01	0.24	17%	0.98	1.18	0.44	0.16	16%
3C10-OLE	C10 3-Alkenes	4.50	0.89	20%	4.62	3%	1.86	0.46	25%	1.21	0.40	33%	1.42	2.08	1.01	0.24	17%	0.98	1.18	0.44	0.16	16%
C10-OLE2	C10 Internal Alkenes	4.50	0.89	20%	4.62	3%	1.86	0.46	25%	1.21	0.40	33%	1.42	2.08	1.01	0.24	17%	0.98	1.18	0.44	0.16	16%
T-5-C11E	Trans-5-Undecene	4.23	0.84	20%	4.31	2%	1.79	0.45	25%	1.17	0.40	34%	1.36	1.90	0.98	0.23	17%	0.91	1.11	0.38	0.16	17%
3C11-OLE	C11 3-Alkenes	4.23	0.84	20%	4.31	2%	1.79	0.45	25%	1.17	0.40	34%	1.36	1.90	0.98	0.23	17%	0.91	1.11	0.38	0.16	17%
C11-OLE2	C11 Internal Alkenes	4.23	0.84	20%	4.31	2%	1.79	0.45	25%	1.17	0.40	34%	1.36	1.90	0.98	0.23	17%	0.91	1.11	0.38	0.16	17%
2C12-OLE	C12 2-Alkenes	3.75	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
3C12-OLE	C12 3-Alkenes	3.75	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
C12-OLE2	C12 Internal Alkenes	3.75	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
T-5-C12E	Trans-5-Dodecene	3.74	0.75	20%	3.87	3%	1.59	0.41	26%	1.04	0.35	34%	1.20	1.64	0.85	0.20	17%	0.79	0.97	0.30	0.15	19%
T-5-C13E	Trans-5-Tridecene	3.38	0.68	20%	3.49	3%	1.43	0.38	26%	0.93	0.32	35%	1.07	1.47	0.78	0.18	16%	0.69	0.87	0.23	0.14	20%
3C13-OLE	C13 3-Alkenes	3.38	0.68	20%	3.49	3%	1.43	0.38	26%	0.93	0.32	35%	1.07	1.47	0.78	0.18	16%	0.69	0.87	0.23	0.14	20%
C13-OLE2	C13 Internal Alkenes	3.38	0.68	20%	3.49	3%	1.43	0.38	26%	0.93	0.32	35%	1.07	1.47	0.78	0.18	16%	0.69	0.87	0.23	0.14	20%
T-5-C14E	Trans-5-Tetradecene	3.08	0.62	20%	3.15	2%	1.31	0.35	27%	0.84	0.30	36%	0.96	1.33	0.68	0.16	16%	0.62	0.79	0.17	0.13	22%
3C14-OLE	C14 3-Alkenes	3.08	0.62	20%	3.15	2%	1.31	0.35	27%	0.84	0.30	36%	0.96	1.33	0.68	0.16	16%	0.62	0.79	0.17	0.13	22%
C14-OLE2	C14 Internal Alkenes	3.08	0.62	20%	3.15	2%	1.31	0.35	27%	0.84	0.30	36%	0.96	1.33	0.68	0.16	16%	0.62	0.79	0.17	0.13	22%
T-5-C15E	Trans-5-Pentadecene	2.82	0.58	20%	2.89	2%	1.20	0.32	27%	0.78	0.28	36%	0.88	1.22	0.63	0.15	17%	0.55	0.71	0.13	0.13	24%
3C15-OLE	C15 3-Alkenes	2.82	0.58	20%	2.89	2%	1.20	0.32	27%	0.78	0.28	36%	0.88	1.22	0.63	0.15	17%	0.55	0.71	0.13	0.13	24%
C15-OLE2	C15 Internal Alkenes	2.82	0.58	20%	2.89	2%	1.20	0.32	27%	0.78	0.28	36%	0.88	1.22	0.63	0.15	17%	0.55	0.71	0.13	0.13	24%
C4-OLE	C4 Alkenes	11.93	1.77	15%	12.35	4%	4.43	0.70	16%	2.78	0.67	24%	3.41	5.57	2.95	0.45	13%	3.65	4.42	3.39	0.20	6%
C5-OLE	C5 Alkenes	9.01	1.51	17%	9.31	3%	3.49	0.65	19%	2.25	0.60	27%	2.71	4.31	2.32	0.37	14%	2.52	2.78	2.26	0.13	5%
C6-OLE	C6 Alkenes	6.88	1.18	17%	7.08	3%	2.75	0.56	20%	1.76	0.50	29%	2.09	3.07	1.78	0.25	12%	1.85	2.06	1.44	0.12	6%
C7-OLE	C7 Alkenes	5.76	1.08	19%	5.92	3%	2.36	0.53	23%	1.53	0.47	31%	1.80	2.59	1.43	0.26	14%	1.42	1.63	1.00	0.13	9%
C8-OLE	C8 Alkenes	4.68	0.89	19%	4.79	2%	1.92	0.45	24%	1.23	0.40	32%	1.44	1.94	1.12	0.20	14%	1.08	1.26	0.66	0.13	12%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
C9-OLE	C9 Alkenes	4.03	0.79	20%	4.14	3%	1.70	0.42	25%	1.09	0.37	34%	1.25	1.67	0.95	0.18	14%	0.88	1.05	0.43	0.14	16%
C10-OLE	C10 Alkenes	3.39	0.68	20%	3.46	2%	1.44	0.38	26%	0.91	0.33	36%	1.04	1.40	0.77	0.16	15%	0.69	0.86	0.25	0.14	20%
C11-OLE	C11 Alkenes	3.09	0.63	20%	3.15	2%	1.33	0.36	27%	0.85	0.31	36%	0.96	1.30	0.71	0.15	16%	0.61	0.79	0.17	0.14	22%
C12-OLE	C12 Alkenes	2.73	0.56	21%	2.80	3%	1.18	0.32	27%	0.75	0.28	37%	0.84	1.14	0.61	0.13	16%	0.52	0.69	0.11	0.13	25%
C13-OLE	C13 Alkenes	2.46	0.51	21%	2.53	3%	1.06	0.30	28%	0.67	0.26	38%	0.75	1.02	0.54	0.12	17%	0.46	0.62	0.06	0.13	28%
C14-OLE	C14 Alkenes	2.28	0.47	21%	2.32	2%	0.98	0.27	28%	0.62	0.23	38%	0.70	0.96	0.50	0.12	17%	0.42	0.57	0.06	0.12	27%
C15-OLE	C15 Alkenes	2.06	0.43	21%	2.10	2%	0.90	0.26	29%	0.56	0.22	40%	0.61	0.85	0.44	0.11	18%	0.36	0.51	0.01	0.12	33%
CYC-PNTE	Cyclopentene	7.38	1.30	18%	7.65	4%	2.81	0.57	20%	1.81	0.52	29%	2.19	3.70	1.70	0.37	17%	1.90	2.23	1.54	0.17	9%
1M-CC5E	1-Methyl cyclopentene	13.95	1.94	14%	14.55	4%	4.87	0.69	14%	2.81	0.68	24%	3.50	5.18	2.72	0.49	14%	4.99	6.24	4.04	0.43	9%
CYC-HEXE	Cyclohexene	5.45	1.04	19%	5.64	4%	2.24	0.50	22%	1.51	0.46	30%	1.79	2.85	1.32	0.34	19%	1.38	1.75	0.91	0.17	12%
1M-CC6E	1-Methyl Cyclohexene	7.81	1.21	16%	8.18	5%	2.89	0.52	18%	1.73	0.47	27%	2.10	2.91	1.76	0.19	9%	2.44	2.91	1.87	0.23	10%
4M-CC6E	4-Methyl Cyclohexene	4.48	0.88	20%	4.61	3%	1.86	0.44	24%	1.25	0.40	32%	1.47	2.26	1.05	0.28	19%	1.07	1.37	0.59	0.16	15%
12M-CC6E	1,2-Dimethyl Cyclohexene	6.77	1.11	16%	7.07	4%	2.56	0.50	19%	1.46	0.43	29%	1.73	2.05	1.42	0.14	8%	2.14	2.45	1.65	0.23	11%
13-BUTDE	1,3-Butadiene	13.58	1.88	14%	13.99	3%	4.83	0.73	15%	2.90	0.70	24%	3.59	5.36	3.10	0.42	12%	4.03	4.85	3.71	0.24	6%
ISOPRENE	Isoprene	10.69	1.62	15%	11.03	3%	3.95	0.64	16%	2.48	0.62	25%	3.01	4.52	2.60	0.36	12%	3.04	3.44	2.77	0.16	5%
C6-OL2D	C6 Cyclic or di-olefins	8.65	1.42	16%	8.94	3%	3.31	0.62	19%	2.11	0.57	27%	2.57	4.16	2.20	0.36	14%	2.43	2.68	2.02	0.14	6%
C7-OL2D	C7 Cyclic or di-olefins	7.49	1.24	17%	7.72	3%	2.95	0.57	19%	1.89	0.52	27%	2.27	3.59	1.91	0.31	14%	2.05	2.27	1.56	0.15	7%
C8-OL2D	C8 Cyclic or di-olefins	6.01	1.15	19%	6.20	3%	2.39	0.55	23%	1.56	0.48	31%	1.85	2.85	1.42	0.31	17%	1.42	1.71	0.90	0.17	12%
C9-OL2D	C9 Cyclic or di-olefins	5.40	1.04	19%	5.56	3%	2.21	0.53	24%	1.45	0.47	32%	1.71	2.53	1.26	0.29	17%	1.23	1.48	0.67	0.17	14%
C10-OL2D	C10 Cyclic or di-olefins	4.56	0.90	20%	4.69	3%	1.89	0.47	25%	1.23	0.41	33%	1.44	2.11	1.03	0.25	17%	0.99	1.20	0.45	0.16	16%
C11-OL2D	C11 Cyclic or di-olefins	4.29	0.85	20%	4.37	2%	1.81	0.46	25%	1.19	0.40	34%	1.37	1.93	0.99	0.23	17%	0.92	1.12	0.38	0.16	17%
C12-OL2D	C12 Cyclic or di-olefins	3.79	0.76	20%	3.91	3%	1.61	0.41	26%	1.05	0.36	34%	1.21	1.66	0.86	0.20	17%	0.80	0.98	0.30	0.15	19%
C13-OL2D	C13 Cyclic or di-olefins	3.42	0.69	20%	3.53	3%	1.45	0.38	26%	0.94	0.33	35%	1.08	1.48	0.79	0.18	16%	0.70	0.88	0.23	0.14	20%
C14-OL2D	C14 Cyclic or di-olefins	3.11	0.63	20%	3.18	2%	1.32	0.35	27%	0.85	0.30	36%	0.97	1.34	0.69	0.16	16%	0.62	0.80	0.17	0.14	22%
C15-OL2D	C15 Cyclic or di-olefins	2.85	0.58	20%	2.91	2%	1.21	0.32	27%	0.78	0.28	36%	0.89	1.23	0.64	0.15	17%	0.56	0.72	0.13	0.13	24%
CYC-PNDE	Cyclopentadiene	7.61	1.34	18%	7.88	4%	2.89	0.59	20%	1.86	0.53	29%	2.26	3.81	1.75	0.38	17%	1.96	2.29	1.59	0.17	9%
3-CARENE	3-Carene	3.21	0.63	19%	3.36	5%	1.27	0.30	24%	0.79	0.26	34%	0.91	1.13	0.64	0.10	11%	0.79	1.00	0.21	0.15	19%
A-PINENE	a-Pinene	4.29	0.68	16%	4.51	5%	1.56	0.29	19%	0.90	0.26	29%	1.08	1.21	0.88	0.08	8%	1.23	1.42	0.76	0.16	13%
B-PINENE	b-Pinene	3.28	0.62	19%	3.39	3%	1.37	0.32	24%	0.83	0.28	34%	0.94	1.12	0.75	0.09	10%	0.82	0.96	0.42	0.11	13%
D-LIMONE	d-Limonene	3.99	0.72	18%	4.19	5%	1.48	0.31	21%	0.89	0.27	30%	1.06	1.25	0.76	0.09	9%	1.15	1.44	0.46	0.19	17%
SABINENE	Sabinene	3.67	0.65	18%	3.81	4%	1.45	0.32	22%	0.84	0.28	34%	0.96	1.10	0.73	0.09	9%	0.97	1.15	0.48	0.14	14%
TERPENE	Terpene	3.79	0.65	17%	3.95	4%	1.45	0.30	21%	0.86	0.27	31%	1.00	1.14	0.78	0.07	7%	1.02	1.21	0.54	0.14	13%
STYRENE	Styrene	1.95	0.39	20%	2.04	5%	-0.62	0.18	-29%	-1.57	0.56	-36%	-1.86	0.53	-9.07	1.78	-96%	-0.59	0.55	-3.01	0.86	-145%
AME-STYR	a-Methyl Styrene	1.72	0.34	20%	1.80	5%	-0.55	0.16	-29%	-1.38	0.50	-36%	-1.64	0.47	-8.00	1.57	-96%	-0.52	0.49	-2.64	0.76	-145%
C9-STYR	C9 Styrenes	1.72	0.34	20%	1.80	5%	-0.55	0.16	-29%	-1.38	0.50	-36%	-1.64	0.47	-8.00	1.57	-96%	-0.52	0.49	-2.64	0.76	-145%
C10-STYR	C10 Styrenes	1.53	0.31	20%	1.61	5%	-0.49	0.14	-29%	-1.24	0.44	-36%	-1.47	0.42	-7.14	1.40	-96%	-0.46	0.43	-2.37	0.68	-145%
BENZENE	Benzene	0.81	0.19	24%	0.82	1%	0.34	0.13	38%	0.16	0.12	74%	0.17	0.28	-0.31	0.11	63%	0.17	0.22	0.05	0.03	19%
TOLUENE	Toluene	3.97	0.72	18%	4.05	2%	1.17	0.32	28%	0.36	0.31	86%	0.44	1.06	-1.79	0.51	116%	0.78	1.01	0.15	0.17	22%
C2-BENZ	Ethyl Benzene	2.79	0.56	20%	2.83	2%	1.00	0.30	30%	0.43	0.27	64%	0.48	0.80	-0.97	0.31	63%	0.58	0.71	0.14	0.10	17%
I-C3-BEN	Isopropyl Benzene (cumene)	2.32	0.47	20%	2.36	2%	0.84	0.26	31%	0.36	0.23	65%	0.40	0.67	-0.83	0.26	65%	0.48	0.59	0.11	0.09	18%
N-C3-BEN	n-Propyl Benzene	2.20	0.45	20%	2.23	1%	0.79	0.25	31%	0.34	0.22	66%	0.38	0.64	-0.81	0.25	67%	0.45	0.56	0.09	0.08	18%
C9-BEN1	C9 Monosub. Benzenes	2.20	0.45	20%	2.23	1%	0.79	0.25	31%	0.34	0.22	66%	0.38	0.64	-0.81	0.25	67%	0.45	0.56	0.09	0.08	18%
S-C4-BEN	s-Butyl Benzene	1.97	0.40	20%	2.00	1%	0.71	0.22	31%	0.30	0.20	66%	0.34	0.57	-0.73	0.22	67%	0.40	0.50	0.08	0.07	18%
C10-BEN1	C10 Monosub. Benzenes	1.97	0.40	20%	2.00	1%	0.71	0.22	31%	0.30	0.20	66%	0.34	0.57	-0.73	0.22	67%	0.40	0.50	0.08	0.07	18%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
N-C4-BEN	n-Butyl Benzene	1.97	0.40	20%	2.00	1%	0.71	0.22	31%	0.30	0.20	66%	0.34	0.57	-0.73	0.22	67%	0.40	0.50	0.08	0.07	18%
C11-BEN1	C11 Monosub. Benzenes	1.78	0.36	20%	1.81	1%	0.64	0.20	31%	0.27	0.18	66%	0.31	0.52	-0.66	0.20	67%	0.36	0.45	0.07	0.07	18%
C12-BEN1	C12 Monosub. Benzenes	1.63	0.33	20%	1.65	1%	0.59	0.18	31%	0.25	0.17	66%	0.28	0.47	-0.60	0.19	67%	0.33	0.42	0.07	0.06	18%
C13-BEN1	C13 Monosub. Benzenes	1.50	0.31	20%	1.52	1%	0.54	0.17	31%	0.23	0.15	66%	0.26	0.44	-0.55	0.17	67%	0.31	0.38	0.06	0.06	18%
M-XYLENE	m-Xylene	10.61	1.49	14%	10.89	3%	3.19	0.47	15%	1.55	0.47	31%	1.95	3.30	0.53	0.51	26%	2.88	3.38	2.26	0.27	9%
O-XYLENE	o-Xylene	7.49	1.19	16%	7.67	2%	2.46	0.46	19%	1.22	0.42	34%	1.50	2.02	0.34	0.32	21%	1.84	2.03	1.57	0.13	7%
P-XYLENE	p-Xylene	4.25	0.75	18%	4.34	2%	1.36	0.35	25%	0.55	0.33	60%	0.63	1.10	-1.47	0.44	70%	0.88	1.07	0.23	0.15	17%
C8-BEN2	C8 Disub. Benzenes	5.16	0.84	16%	5.28	2%	1.68	0.35	21%	0.77	0.33	43%	0.93	1.37	-0.58	0.34	37%	1.24	1.37	0.84	0.12	10%
C9-BEN2	C9 Disub. Benzenes	6.61	1.00	15%	6.76	2%	2.07	0.37	18%	0.98	0.35	36%	1.21	1.88	-0.17	0.36	29%	1.66	1.88	1.34	0.14	9%
C10-BEN2	C10 Disub. Benzenes	5.92	0.90	15%	6.04	2%	1.85	0.33	18%	0.88	0.32	36%	1.08	1.69	-0.15	0.32	29%	1.49	1.68	1.20	0.13	9%
C11-BEN2	C11 Disub. Benzenes	5.35	0.81	15%	5.49	2%	1.68	0.30	18%	0.79	0.29	36%	0.98	1.53	-0.14	0.29	30%	1.35	1.52	1.09	0.12	9%
C12-BEN2	C12 Disub. Benzenes	4.90	0.74	15%	5.01	2%	1.53	0.27	18%	0.73	0.26	36%	0.89	1.39	-0.13	0.26	30%	1.23	1.39	0.99	0.11	9%
C13-BEN2	C13 Disub. Benzenes	4.50	0.68	15%	4.60	2%	1.41	0.25	18%	0.67	0.24	36%	0.82	1.28	-0.12	0.24	29%	1.13	1.28	0.91	0.10	9%
C8-BEN2	Isomers of Ethylbenzene	5.16	0.84	16%	5.28	2%	1.68	0.35	21%	0.77	0.33	43%	0.93	1.37	-0.58	0.34	37%	1.24	1.37	0.84	0.12	10%
123-TMB	1,2,3-Trimethyl Benzene	11.26	1.58	14%	11.57	3%	3.49	0.50	14%	1.81	0.49	27%	2.28	3.57	1.63	0.41	18%	3.12	3.70	2.51	0.26	8%
124-TMB	1,2,4-Trimethyl Benzene	7.18	1.09	15%	7.37	3%	2.32	0.41	18%	1.18	0.39	33%	1.44	2.14	0.27	0.30	21%	1.83	2.15	1.45	0.14	8%
135-TMB	1,3,5-Trimethyl Benzene	11.22	1.55	14%	11.57	3%	3.44	0.44	13%	1.80	0.46	26%	2.29	3.74	1.68	0.42	18%	3.34	4.07	2.70	0.30	9%
C9-BEN	Isomers of Propylbenzene	6.12	0.91	15%	6.29	3%	1.96	0.33	17%	0.98	0.32	33%	1.21	1.83	0.24	0.27	22%	1.63	1.89	1.34	0.12	8%
C9-BEN3	C9 Trisub. Benzenes	9.90	1.40	14%	10.17	3%	3.09	0.44	14%	1.60	0.44	28%	2.00	3.14	1.26	0.36	18%	2.77	3.32	2.26	0.23	8%
C10-BEN	Isomers of Butylbenzene	5.48	0.82	15%	5.62	3%	1.76	0.30	17%	0.88	0.29	33%	1.08	1.64	0.22	0.24	22%	1.46	1.69	1.20	0.11	8%
C10-BEN4	C10 Tetrasub. Benzenes	8.86	1.26	14%	9.12	3%	2.76	0.40	14%	1.43	0.40	28%	1.79	2.82	1.13	0.32	18%	2.48	2.97	2.02	0.20	8%
C10-BEN3	C10 Trisub. Benzenes	8.86	1.26	14%	9.12	3%	2.76	0.40	14%	1.43	0.40	28%	1.79	2.82	1.13	0.32	18%	2.48	2.97	2.02	0.20	8%
C11-BEN	Isomers of Pentylbenzene	4.96	0.74	15%	5.09	3%	1.59	0.27	17%	0.79	0.26	33%	0.98	1.48	0.20	0.22	22%	1.32	1.54	1.09	0.10	8%
C11-BEN5	C11 Pentasub. Benzenes	8.03	1.14	14%	8.26	3%	2.50	0.36	14%	1.30	0.36	28%	1.63	2.56	1.02	0.29	18%	2.24	2.69	1.83	0.18	8%
C11-BEN4	C11 Tetrasub. Benzenes	8.03	1.14	14%	8.26	3%	2.50	0.36	14%	1.30	0.36	28%	1.63	2.56	1.02	0.29	18%	2.24	2.69	1.83	0.18	8%
C11-BEN3	C11 Trisub. Benzenes	8.03	1.14	14%	8.26	3%	2.50	0.36	14%	1.30	0.36	28%	1.63	2.56	1.02	0.29	18%	2.24	2.69	1.83	0.18	8%
C12-BEN	Isomers of Hexylbenzene	4.53	0.68	15%	4.65	3%	1.45	0.25	17%	0.72	0.24	33%	0.89	1.35	0.18	0.20	22%	1.21	1.40	1.00	0.09	8%
C12-BEN5	C11 Pentasub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C12-BEN6	C12 Hexaasub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C12-BEN4	C12 Tetrasub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C12-BEN3	C12 Trisub. Benzenes	7.33	1.04	14%	7.53	3%	2.29	0.33	14%	1.18	0.33	28%	1.49	2.34	0.93	0.27	18%	2.05	2.46	1.67	0.17	8%
C13-BEN3	C13 Trisub. Benzenes	6.75	0.96	14%	6.94	3%	2.10	0.30	14%	1.09	0.30	28%	1.37	2.14	0.86	0.24	18%	1.89	2.26	1.54	0.15	8%
INDAN	Indan	3.17	0.48	15%	3.26	3%	0.41	0.29	70%	-0.39	0.42	-109%	-0.46	0.83	-5.80	1.13	-	0.29	0.84	-1.68	0.49	170%
NAPHTHAL	Naphthalene	3.26	0.57	17%	3.35	3%	1.02	0.27	27%	0.44	0.27	60%	0.53	0.84	-0.96	0.31	60%	0.68	0.82	0.07	0.14	21%
TETRALIN	Tetralin	2.83	0.43	15%	2.91	3%	0.37	0.26	70%	-0.35	0.38	-109%	-0.41	0.75	-5.18	1.01	-	0.26	0.75	-1.51	0.43	170%
ME-NAPH	Methyl Naphthalenes	4.61	0.69	15%	4.75	3%	1.33	0.23	17%	0.55	0.24	44%	0.70	1.39	-0.77	0.35	50%	1.13	1.47	0.51	0.20	17%
1ME-NAPH	1-Methyl Naphthalene	4.61	0.69	15%	4.75	3%	1.33	0.23	17%	0.55	0.24	44%	0.70	1.39	-0.77	0.35	50%	1.13	1.47	0.51	0.20	17%
2ME-NAPH	2-Methyl Naphthalene	4.61	0.69	15%	4.75	3%	1.33	0.23	17%	0.55	0.24	44%	0.70	1.39	-0.77	0.35	50%	1.13	1.47	0.51	0.20	17%
C11-TET	C11 Tetralin or Indane	2.56	0.39	15%	2.63	3%	0.33	0.23	70%	-0.31	0.34	-109%	-0.37	0.67	-4.68	0.91	-	0.23	0.68	-1.37	0.39	170%
23-DMN	2,3-Dimethyl Naphth.	5.54	0.80	15%	5.72	3%	1.61	0.24	15%	0.73	0.25	34%	0.94	1.74	-0.13	0.32	34%	1.52	1.92	1.00	0.20	13%
C12-NAP2	C12 Disub. Naphthalenes	5.54	0.80	15%	5.72	3%	1.61	0.24	15%	0.73	0.25	34%	0.94	1.74	-0.13	0.32	34%	1.52	1.92	1.00	0.20	13%
DM-NAPH	Dimethyl Naphthalenes	5.54	0.80	15%	5.72	3%	1.61	0.24	15%	0.73	0.25	34%	0.94	1.74	-0.13	0.32	34%	1.52	1.92	1.00	0.20	13%
C12-NAP1	C12 Monosub. Naphth.	4.20	0.63	15%	4.31	3%	1.21	0.21	17%	0.50	0.22	44%	0.64	1.26	-0.70	0.32	50%	1.03	1.34	0.47	0.18	18%
C13-NAP2	C13 Disub. Naphthalenes	5.08	0.73	14%	5.24	3%	1.47	0.22	15%	0.67	0.23	34%	0.86	1.59	-0.12	0.29	34%	1.39	1.76	0.92	0.18	13%
C13-NAP3	C13 Trisub. Naphthalenes	5.08	0.73	14%	5.24	3%	1.47	0.22	15%	0.67	0.23	34%	0.86	1.59	-0.12	0.29	34%	1.39	1.76	0.92	0.18	13%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
C13-NAP1	C13 Monosub. Naphth.	3.86	0.58	15%	3.96	3%	1.11	0.19	17%	0.46	0.20	44%	0.59	1.16	-0.65	0.29	50%	0.95	1.23	0.43	0.17	18%
ACETYLEN	Acetylene	1.25	0.22	18%	1.26	1%	0.49	0.10	20%	0.28	0.08	29%	0.34	0.47	0.28	0.04	12%	0.30	0.38	0.27	0.03	9%
ME-ACTYL	Methyl Acetylene	6.45	1.15	18%	6.58	2%	2.35	0.49	21%	1.38	0.42	30%	1.68	2.41	1.08	0.19	11%	1.44	1.68	1.08	0.12	8%
2-BUTYNE	2-Butyne	16.33	2.36	14%	16.72	2%	5.30	0.76	14%	3.08	0.71	23%	3.90	6.48	3.03	0.64	17%	4.38	5.26	3.61	0.40	9%
ET-ACTYL	Ethyl Acetylene	6.20	1.20	19%	6.28	1%	2.39	0.61	25%	1.43	0.52	36%	1.68	2.21	0.70	0.26	15%	1.32	1.60	0.86	0.15	12%
MEOH	Methanol	0.71	0.14	19%	0.72	1%	0.34	0.06	18%	0.22	0.05	25%	0.26	0.44	0.16	0.05	21%	0.21	0.30	0.14	0.03	15%
ETOH	Ethanol	1.69	0.42	25%	1.71	1%	0.93	0.27	29%	0.65	0.23	35%	0.73	1.16	0.31	0.17	24%	0.45	0.66	0.27	0.08	18%
I-C3-OH	Isopropyl Alcohol	0.71	0.14	19%	0.72	1%	0.39	0.07	18%	0.28	0.07	23%	0.33	0.63	0.15	0.09	27%	0.26	0.41	0.14	0.06	22%
N-C3-OH	n-Propyl Alcohol	2.74	0.65	24%	2.76	1%	1.39	0.41	30%	0.94	0.35	37%	1.05	1.52	0.56	0.23	22%	0.67	0.95	0.48	0.10	15%
I-C4-OH	Isobutyl Alcohol	2.24	0.48	22%	2.26	1%	1.10	0.28	26%	0.73	0.24	33%	0.83	1.24	0.48	0.15	18%	0.58	0.75	0.44	0.07	11%
N-C4-OH	n-Butyl Alcohol	3.34	0.74	22%	3.37	1%	1.62	0.44	27%	1.09	0.38	35%	1.24	1.82	0.73	0.25	20%	0.84	1.14	0.66	0.11	13%
S-C4-OH	s-Butyl Alcohol	1.60	0.35	22%	1.62	2%	0.84	0.21	25%	0.59	0.18	30%	0.67	1.11	0.33	0.14	21%	0.48	0.66	0.30	0.08	17%
T-C4-OH	t-Butyl Alcohol	0.45	0.09	20%	0.46	1%	0.25	0.05	19%	0.17	0.04	26%	0.19	0.34	0.09	0.05	25%	0.14	0.21	0.08	0.03	18%
CC5-OH	Cyclopentanol	1.96	0.42	21%	1.98	1%	0.99	0.25	25%	0.68	0.21	31%	0.77	1.19	0.42	0.15	20%	0.55	0.74	0.39	0.08	14%
2-C5OH	2-Pentanol	1.74	0.36	21%	1.76	1%	0.89	0.22	25%	0.61	0.19	31%	0.69	1.11	0.37	0.14	20%	0.50	0.69	0.34	0.08	15%
3-C5OH	3-Pentanol	1.73	0.38	22%	1.77	2%	0.88	0.22	25%	0.61	0.19	32%	0.69	1.10	0.37	0.14	20%	0.49	0.66	0.34	0.07	15%
C5OH	Pentyl Alcohol	3.35	0.73	22%	3.40	2%	1.60	0.42	27%	1.08	0.37	34%	1.22	1.79	0.74	0.24	19%	0.84	1.10	0.67	0.10	12%
CC6-OH	Cyclohexanol	2.25	0.52	23%	2.27	1%	1.20	0.33	27%	0.81	0.28	34%	0.89	1.21	0.43	0.17	19%	0.61	0.78	0.40	0.09	14%
1-C6OH	1-Hexanol	2.74	0.61	22%	2.77	1%	1.36	0.37	27%	0.91	0.31	34%	1.02	1.40	0.58	0.19	19%	0.69	0.87	0.53	0.09	13%
2-C6OH	2-Hexanol	2.46	0.60	24%	2.48	0%	1.37	0.38	28%	0.93	0.32	34%	1.03	1.53	0.43	0.22	21%	0.66	0.89	0.38	0.11	17%
1-C7OH	1-Heptanol	2.21	0.51	23%	2.23	1%	1.12	0.32	28%	0.73	0.27	37%	0.80	1.09	0.45	0.15	18%	0.52	0.68	0.39	0.07	14%
1-C8-OH	1-Octanol	2.01	0.48	24%	2.05	2%	1.02	0.31	30%	0.66	0.26	40%	0.71	0.97	0.38	0.15	21%	0.43	0.62	0.22	0.09	21%
2-ETC6OH	2-Ethyl-1-Hexanol	2.20	0.49	22%	2.23	1%	1.08	0.31	28%	0.69	0.26	37%	0.76	1.02	0.46	0.13	17%	0.50	0.64	0.36	0.06	13%
2-C8-OH	2-Octanol	2.16	0.51	23%	2.19	1%	1.13	0.33	29%	0.73	0.27	38%	0.79	1.06	0.41	0.15	20%	0.50	0.70	0.30	0.09	18%
3-C8-OH	3-Octanol	2.57	0.59	23%	2.61	2%	1.28	0.37	29%	0.85	0.32	37%	0.93	1.29	0.53	0.18	19%	0.59	0.79	0.36	0.10	17%
4-C8-OH	4-Octanol	3.07	0.70	23%	3.13	2%	1.49	0.42	28%	0.98	0.36	37%	1.09	1.53	0.65	0.21	19%	0.69	0.89	0.41	0.11	16%
I-C10-OH	8-Methyl-1-Nonanol (Isodecyl Alcohol)	1.18	0.33	28%	1.21	2%	0.63	0.21	34%	0.38	0.18	46%	0.39	0.57	0.09	0.12	30%	0.20	0.33	-0.03	0.08	42%
ET-GLYCL	Ethylene Glycol	3.36	0.70	21%	3.43	2%	1.57	0.35	22%	1.08	0.31	29%	1.27	2.19	0.76	0.26	21%	0.90	1.22	0.69	0.13	14%
PR-GLYCL	Propylene Glycol	2.75	0.52	19%	2.80	2%	1.23	0.28	22%	0.83	0.24	29%	0.97	1.57	0.67	0.17	18%	0.76	0.98	0.63	0.08	11%
12-C4OH2	1,2-Butandiol	2.21	0.44	20%	2.24	1%	1.03	0.24	23%	0.69	0.21	30%	0.80	1.29	0.51	0.15	18%	0.60	0.79	0.47	0.07	12%
GLYCERL	Glycerol	3.27	0.65	20%	3.33	2%	1.41	0.33	23%	0.91	0.28	31%	1.07	1.62	0.74	0.17	16%	0.81	1.04	0.64	0.08	10%
C6-GLYCL	1,2-Dihydroxy Hexane	2.75	0.57	21%	2.78	1%	1.28	0.32	25%	0.84	0.27	32%	0.97	1.43	0.58	0.16	17%	0.69	0.88	0.52	0.08	11%
2M24C5OH	2-Methyl-2,4-Pentanediol	1.04	0.21	20%	1.05	0%	0.53	0.13	25%	0.36	0.11	31%	0.41	0.65	0.22	0.08	19%	0.30	0.40	0.20	0.04	14%
ME-O-ME	Dimethyl Ether	0.93	0.18	19%	0.95	2%	0.58	0.09	16%	0.44	0.09	21%	0.52	1.11	0.18	0.18	34%	0.40	0.68	0.18	0.11	27%
TME-OX	Trimethylene Oxide	5.22	1.18	23%	5.33	2%	2.74	0.66	24%	2.01	0.61	30%	2.32	4.21	1.06	0.61	26%	1.59	2.50	1.00	0.33	21%
THF	Tetrahydrofuran	4.95	1.03	21%	5.03	2%	2.40	0.57	24%	1.67	0.51	30%	1.91	3.01	1.13	0.38	20%	1.43	2.03	1.07	0.21	15%
ET-O-ET	Diethyl Ether	4.01	0.68	17%	4.12	3%	1.86	0.30	16%	1.26	0.29	23%	1.48	2.64	1.00	0.29	19%	1.33	1.92	0.97	0.21	16%
METHYLAL	Dimethoxy methane	1.04	0.20	19%	1.06	2%	0.66	0.11	16%	0.50	0.11	21%	0.59	1.26	0.20	0.20	34%	0.45	0.76	0.19	0.12	27%
AM-THF	Alpha-Methyltetrahyd-rofuran	4.62	0.92	20%	4.74	2%	2.17	0.50	23%	1.48	0.45	30%	1.70	2.48	1.11	0.30	18%	1.30	1.82	1.06	0.17	13%
THP	Tetrahydropyran	3.81	0.81	21%	3.87	2%	1.96	0.46	24%	1.34	0.41	30%	1.51	2.24	0.81	0.28	19%	1.12	1.58	0.75	0.17	15%
ET-O-IPR	Ethyl Isopropyl Ether	3.86	0.63	16%	3.98	3%	1.66	0.26	16%	1.10	0.26	23%	1.30	2.12	1.04	0.21	16%	1.25	1.71	1.04	0.16	13%
MNBE	Methyl n-Butyl Ether	3.66	0.76	21%	3.73	2%	1.81	0.42	23%	1.26	0.38	30%	1.43	2.23	0.81	0.28	20%	1.06	1.49	0.76	0.15	15%
MTBE	Methyl t-Butyl Ether	0.78	0.17	21%	0.79	2%	0.47	0.10	21%	0.32	0.09	27%	0.36	0.64	0.15	0.09	24%	0.26	0.38	0.14	0.05	19%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]									
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
PR-O-PR	Di n-Propyl Ether	3.24	0.65	20%	3.33	3%	1.62	0.36	22%	1.13	0.32	28%	1.29	2.08	0.72	0.25	20%	0.97	1.42	0.67	0.15	15%
ENBE	Ethyl n-Butyl Ether	3.86	0.73	19%	3.95	2%	1.80	0.39	22%	1.21	0.35	29%	1.39	2.12	0.93	0.23	17%	1.11	1.51	0.89	0.13	12%
ETBE	Ethyl t-Butyl Ether	2.11	0.39	18%	2.16	2%	1.04	0.18	17%	0.69	0.17	24%	0.80	1.35	0.48	0.15	18%	0.67	0.93	0.46	0.10	15%
MTAE	Methyl t-Amyl Ether	2.14	0.44	20%	2.19	2%	1.11	0.23	20%	0.75	0.20	27%	0.86	1.40	0.45	0.16	18%	0.65	0.88	0.42	0.09	14%
2BU-THF	2-Butyl Tetrahydrofuran	2.53	0.60	24%	2.59	2%	1.22	0.36	30%	0.79	0.31	39%	0.86	1.20	0.54	0.18	21%	0.50	0.77	0.08	0.14	28%
IBU2-O	Di-Isobutyl Ether	1.29	0.32	24%	1.34	3%	0.69	0.19	27%	0.46	0.16	35%	0.49	0.73	0.25	0.10	20%	0.36	0.54	0.21	0.08	21%
BU-O-BU	Di-n-butyl Ether	3.17	0.67	21%	3.24	2%	1.50	0.39	26%	1.01	0.34	34%	1.13	1.53	0.74	0.20	17%	0.79	1.05	0.51	0.11	14%
C5-O-C5	Di-n-Pentyl Ether	2.64	0.63	24%	2.69	2%	1.36	0.40	29%	0.91	0.34	37%	0.99	1.35	0.53	0.19	20%	0.61	0.89	0.29	0.13	21%
MEO-ETOH	2-Methoxyethanol	2.98	0.48	16%	3.05	2%	1.30	0.21	16%	0.87	0.20	23%	1.04	1.87	0.78	0.20	19%	0.95	1.33	0.76	0.13	13%
MEOC3OH	1-Methoxy-2-Propanol	2.62	0.51	19%	2.68	3%	1.28	0.26	21%	0.90	0.24	26%	1.05	1.87	0.58	0.23	22%	0.81	1.16	0.55	0.13	16%
ETO-ETOH	2-Ethoxyethanol	3.78	0.64	17%	3.86	2%	1.65	0.30	18%	1.09	0.27	25%	1.29	2.16	0.98	0.21	16%	1.15	1.54	0.95	0.13	11%
2MEOC3OH	2-Methoxy-1-Propanol	3.01	0.41	14%	3.09	2%	1.18	0.15	13%	0.75	0.16	21%	0.91	1.52	0.77	0.15	16%	0.98	1.35	0.86	0.11	11%
ETOC3OH	1-Ethoxy-2-Propanol	3.25	0.59	18%	3.32	2%	1.52	0.30	19%	1.04	0.27	26%	1.21	2.02	0.76	0.23	19%	0.99	1.36	0.73	0.13	14%
2PROETOH	2-Propoxyethanol	3.52	0.63	18%	3.60	2%	1.60	0.33	20%	1.08	0.29	27%	1.25	2.01	0.87	0.21	17%	1.05	1.41	0.84	0.12	12%
3ETOC3OH	3-Ethoxy-1-Propanol	4.24	0.70	16%	4.33	2%	1.82	0.32	18%	1.19	0.30	25%	1.40	2.24	1.13	0.20	14%	1.27	1.65	1.11	0.13	10%
3MEOC4OH	3-Methoxy-1-Butanol	0.97	0.19	20%	0.98	1%	0.52	0.10	20%	0.35	0.09	26%	0.41	0.72	0.20	0.09	22%	0.31	0.43	0.19	0.05	17%
DET-GLCL	Diethylene Glycol	3.55	0.61	17%	3.62	2%	1.53	0.30	20%	1.00	0.27	27%	1.17	1.82	0.94	0.17	14%	1.05	1.33	0.93	0.10	9%
PROXC3OH	1-Propoxy-2-Propanol	2.86	0.57	20%	2.92	2%	1.41	0.31	22%	0.97	0.28	28%	1.12	1.84	0.62	0.22	20%	0.84	1.20	0.58	0.12	15%
BUO-ETOH	2-Butoxyethanol	2.90	0.52	18%	2.95	2%	1.28	0.28	22%	0.83	0.25	30%	0.96	1.35	0.73	0.12	13%	0.80	0.98	0.70	0.06	8%
3MOMC4OH	3 methoxy -3 methyl-Butanol	1.74	0.37	22%	1.76	1%	0.88	0.23	26%	0.59	0.19	33%	0.66	1.00	0.37	0.12	18%	0.46	0.59	0.34	0.06	12%
MOEOETOH	2-(2-Methoxyethoxy) Ethanol	2.90	0.51	18%	2.96	2%	1.35	0.26	19%	0.93	0.24	26%	1.08	1.79	0.71	0.20	19%	0.97	1.38	0.72	0.14	15%
PG-1TB-E	1-tert-Butoxy-2-Propanol	1.71	0.37	21%	1.74	1%	0.88	0.22	26%	0.59	0.19	32%	0.66	0.95	0.35	0.12	18%	0.45	0.60	0.31	0.06	13%
PG-2TB-E	2-tert-Butoxy-1-Propanol	1.81	0.26	14%	1.84	2%	0.71	0.11	16%	0.43	0.11	24%	0.51	0.77	0.45	0.05	10%	0.51	0.63	0.46	0.03	6%
BUOC3OH	n-Butoxy-2-Propanol	2.70	0.56	21%	2.75	2%	1.31	0.32	24%	0.89	0.28	32%	1.01	1.47	0.60	0.18	18%	0.72	0.99	0.55	0.10	13%
CARBITOL	2-(2-Ethoxyethoxy) EtOH	3.19	0.59	19%	3.26	2%	1.47	0.31	21%	0.99	0.28	29%	1.14	1.64	0.76	0.18	16%	0.97	1.35	0.76	0.12	12%
DPR-GLCL	Dipropylene Glycol	2.48	0.51	20%	2.53	2%	1.23	0.28	23%	0.85	0.25	29%	0.96	1.51	0.52	0.19	19%	0.72	1.00	0.48	0.10	14%
EGHE	2-Hexyloxyethanol	2.45	0.52	21%	2.50	2%	1.20	0.32	26%	0.78	0.27	35%	0.86	1.12	0.53	0.14	16%	0.61	0.80	0.44	0.08	13%
DGPE	2-(2-Propoxyethoxy) ethanol	3.00	0.58	19%	3.06	2%	1.42	0.32	22%	0.96	0.28	29%	1.09	1.60	0.69	0.18	17%	0.87	1.22	0.67	0.11	13%
DPRGOME	Dipropylene Glycol Methyl Ether	2.21	0.41	18%	2.26	3%	1.05	0.21	20%	0.73	0.19	27%	0.83	1.25	0.49	0.15	18%	0.71	1.06	0.48	0.11	16%
C8-CELSV	2-(2-Butoxyethoxy)-EtOH	2.70	0.55	20%	2.77	3%	1.28	0.31	24%	0.86	0.27	32%	0.97	1.27	0.61	0.15	16%	0.72	0.98	0.53	0.09	13%
TGME	2-[2-(2-Methoxyethoxy) ethoxy] ethanol	2.62	0.51	19%	2.66	2%	1.26	0.27	22%	0.86	0.25	28%	0.98	1.42	0.58	0.17	17%	0.83	1.22	0.57	0.13	15%
EGEHE	2-(2-Ethylhexyloxy) ethanol	1.71	0.44	26%	1.74	2%	0.89	0.29	33%	0.56	0.25	44%	0.58	0.81	0.24	0.15	27%	0.32	0.53	0.02	0.11	36%
TGEE	2-[2-(2-Ethoxyethoxy) ethoxy] ethanol	2.66	0.54	20%	2.74	3%	1.28	0.30	23%	0.86	0.26	31%	0.97	1.29	0.58	0.16	16%	0.77	1.11	0.55	0.11	15%
DGHE	2-(2-Hexyloxyethoxy) ethanol	2.03	0.48	23%	2.07	2%	1.03	0.29	28%	0.68	0.25	37%	0.73	0.98	0.40	0.14	19%	0.47	0.69	0.21	0.10	21%
TGPE	2-[2-(2-Propoxyethoxy) ethoxy] ethanol	2.46	0.52	21%	2.52	2%	1.19	0.30	25%	0.80	0.26	33%	0.90	1.16	0.52	0.15	17%	0.66	0.97	0.41	0.11	16%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
TGBE	2-[2-(2-Butoxyethoxy) ethoxy] ethanol	2.24	0.49	22%	2.29	2%	1.09	0.29	27%	0.73	0.25	35%	0.80	1.07	0.47	0.14	18%	0.55	0.79	0.25	0.10	18%
TPRGOME	Tripropylene Glycol Monomethyl Ether	1.90	0.41	21%	1.95	3%	0.93	0.23	25%	0.62	0.20	33%	0.69	0.91	0.39	0.12	17%	0.52	0.80	0.25	0.11	20%
TETRAGME	2,5,8,11-Tetraoxatridecan-13-ol	2.15	0.47	22%	2.20	2%	1.07	0.26	25%	0.72	0.23	32%	0.80	1.06	0.44	0.14	18%	0.61	0.94	0.36	0.11	18%
TETRAGBE	3,6,9,12-Tetraoxahexa-decan-1-ol	1.90	0.45	24%	1.94	2%	0.94	0.27	29%	0.63	0.23	37%	0.68	0.93	0.37	0.14	20%	0.43	0.68	0.07	0.11	27%
ME-FORM	Methyl Formate	0.07	0.01	21%	0.07	2%	0.05	0.01	20%	0.04	0.01	24%	0.04	0.09	0.01	0.01	36%	0.03	0.05	0.01	0.01	29%
ET-FORM	Ethyl Formate	0.52	0.13	25%	0.53	2%	0.31	0.09	29%	0.23	0.08	35%	0.26	0.44	0.10	0.07	27%	0.15	0.24	0.09	0.03	22%
ME-ACET	Methyl Acetate	0.07	0.02	22%	0.07	2%	0.05	0.01	20%	0.04	0.01	25%	0.05	0.10	0.01	0.02	36%	0.03	0.05	0.01	0.01	29%
ET-ACET	Ethyl Acetate	0.64	0.15	24%	0.65	1%	0.37	0.10	28%	0.26	0.09	34%	0.29	0.48	0.12	0.07	24%	0.18	0.26	0.11	0.03	19%
ME-PRAT	Methyl Propionate	0.71	0.16	23%	0.71	1%	0.35	0.10	28%	0.22	0.08	36%	0.25	0.34	0.14	0.04	16%	0.17	0.22	0.13	0.02	10%
C3-FORM	n-Propyl Formate	0.93	0.26	28%	0.93	1%	0.55	0.19	34%	0.39	0.16	41%	0.43	0.66	0.15	0.12	29%	0.23	0.36	0.13	0.06	25%
ET-PRAT	Ethyl Propionate	0.79	0.19	24%	0.80	1%	0.44	0.13	29%	0.30	0.11	35%	0.34	0.52	0.15	0.07	22%	0.21	0.29	0.13	0.04	17%
IPR-ACET	Isopropyl Acetate	1.24	0.23	18%	1.25	1%	0.65	0.12	18%	0.44	0.11	24%	0.51	0.89	0.27	0.11	21%	0.40	0.56	0.25	0.07	16%
ME-BUAT	Methyl Butyrate	1.18	0.26	22%	1.19	1%	0.60	0.16	26%	0.38	0.13	34%	0.43	0.61	0.23	0.07	16%	0.31	0.39	0.21	0.03	11%
ME-IBUAT	Methyl Isobutyrate	0.70	0.18	25%	0.71	1%	0.40	0.12	31%	0.27	0.10	39%	0.29	0.43	0.13	0.07	23%	0.18	0.25	0.11	0.03	18%
C4-FORM	n-Butyl Formate	0.95	0.25	27%	0.96	1%	0.57	0.18	32%	0.40	0.16	38%	0.44	0.65	0.16	0.11	26%	0.25	0.37	0.14	0.06	22%
PR-ACET	Propyl Acetate	0.87	0.23	26%	0.88	1%	0.52	0.16	31%	0.36	0.14	37%	0.40	0.60	0.15	0.10	25%	0.23	0.33	0.13	0.05	21%
ET-BUAT	Ethyl Butyrate	1.25	0.28	22%	1.27	1%	0.65	0.17	26%	0.43	0.14	33%	0.48	0.72	0.24	0.08	18%	0.32	0.40	0.22	0.04	13%
IBU-ACET	Isobutyl Acetate	0.67	0.15	22%	0.69	2%	0.43	0.09	20%	0.30	0.08	26%	0.34	0.59	0.12	0.09	26%	0.25	0.36	0.11	0.05	21%
ME-PVAT	Methyl Pivalate	0.41	0.11	26%	0.41	1%	0.24	0.07	30%	0.16	0.06	37%	0.17	0.23	0.07	0.04	20%	0.10	0.14	0.06	0.02	16%
BU-ACET	n-Butyl Acetate	0.89	0.23	26%	0.90	1%	0.54	0.16	31%	0.37	0.14	37%	0.40	0.55	0.15	0.09	23%	0.24	0.32	0.13	0.04	18%
PR-PRAT	n-Propyl Propionate	0.93	0.24	26%	0.93	1%	0.53	0.17	32%	0.36	0.14	39%	0.39	0.57	0.16	0.09	23%	0.23	0.30	0.14	0.05	20%
SBU-ACET	s-Butyl Acetate	1.43	0.34	24%	1.46	2%	0.81	0.20	25%	0.57	0.17	31%	0.64	1.07	0.27	0.14	22%	0.42	0.60	0.24	0.07	17%
TBU-ACET	t-Butyl Acetate	0.22	0.04	20%	0.22	1%	0.13	0.03	21%	0.08	0.02	28%	0.09	0.16	0.04	0.02	21%	0.07	0.10	0.04	0.01	15%
BU-PRAT	Butyl Propionate	0.89	0.23	26%	0.89	0%	0.52	0.16	32%	0.34	0.14	40%	0.36	0.50	0.14	0.08	22%	0.21	0.30	0.12	0.04	19%
AM-ACET	Amyl Acetate	0.96	0.25	26%	0.96	0%	0.59	0.18	31%	0.38	0.15	39%	0.40	0.53	0.15	0.09	23%	0.24	0.35	0.12	0.05	19%
PR-BUAT	n-Propyl Butyrate	1.17	0.29	25%	1.18	1%	0.63	0.19	30%	0.42	0.16	37%	0.46	0.64	0.21	0.10	21%	0.27	0.37	0.18	0.05	19%
23MC4ACT	2,3-Dimethylbutyl Acetate	0.84	0.21	25%	0.85	2%	0.50	0.13	27%	0.33	0.11	34%	0.35	0.55	0.14	0.07	22%	0.23	0.34	0.13	0.04	18%
2MC5-ACT	2-Methylpentyl Acetate	1.11	0.30	27%	1.13	2%	0.64	0.20	32%	0.40	0.17	42%	0.42	0.56	0.17	0.10	24%	0.24	0.37	0.09	0.06	23%
3MC5-ACT	3-Methylpentyl Acetate	1.31	0.35	27%	1.33	1%	0.75	0.23	31%	0.48	0.19	40%	0.51	0.69	0.22	0.11	22%	0.30	0.43	0.17	0.06	19%
4MC5-ACT	4-Methylpentyl Acetate	0.92	0.26	28%	0.94	2%	0.53	0.17	33%	0.34	0.14	43%	0.35	0.48	0.12	0.09	26%	0.19	0.31	0.05	0.05	29%
IBU-IBTR	Isobutyl Isobutyrate	0.64	0.16	26%	0.65	2%	0.39	0.11	27%	0.25	0.09	35%	0.27	0.43	0.11	0.06	23%	0.17	0.25	0.09	0.03	18%
BU-BUAT	n-Butyl Butyrate	1.12	0.28	25%	1.13	1%	0.61	0.19	31%	0.39	0.16	40%	0.42	0.56	0.19	0.09	21%	0.25	0.36	0.13	0.05	22%
NC6-ACET	n-Hexyl Acetate	0.87	0.26	30%	0.88	1%	0.55	0.19	34%	0.33	0.15	45%	0.33	0.48	0.02	0.11	32%	0.18	0.31	0.02	0.06	31%
E3EOC3OH	Ethyl 3-Ethoxy Propionate	3.61	0.59	16%	3.68	2%	1.47	0.27	19%	0.91	0.25	27%	1.08	1.49	0.95	0.09	9%	0.97	1.11	0.91	0.04	4%
24MC5ACT	2,4-Dimethylpentyl Acetate	0.98	0.27	28%	1.00	2%	0.56	0.18	33%	0.33	0.15	45%	0.33	0.48	-0.02	0.11	33%	0.18	0.31	-0.02	0.07	38%
2MC6-ACT	2-Methylhexyl Acetate	0.89	0.27	31%	0.91	2%	0.54	0.19	35%	0.32	0.16	48%	0.32	0.48	-0.04	0.12	37%	0.16	0.29	-0.05	0.07	44%
3EC5-ACT	3-Ethylpentyl Acetate	1.24	0.34	28%	1.26	2%	0.70	0.23	33%	0.44	0.19	43%	0.46	0.62	0.19	0.11	25%	0.25	0.39	0.08	0.06	26%
3MC6-ACT	3-Methylhexyl Acetate	1.01	0.30	29%	1.03	2%	0.59	0.20	35%	0.36	0.17	46%	0.36	0.52	0.03	0.11	31%	0.19	0.32	-0.01	0.07	36%
4MC6-ACT	4-Methylhexyl Acetate	0.91	0.27	30%	0.93	2%	0.53	0.18	35%	0.32	0.15	47%	0.32	0.47	0.02	0.11	34%	0.15	0.28	-0.05	0.07	47%
5MC6-ACT	5-Methylhexyl Acetate	0.79	0.25	32%	0.81	2%	0.49	0.18	37%	0.29	0.15	51%	0.28	0.43	-0.10	0.12	43%	0.13	0.26	-0.08	0.07	53%
IC5IBUAT	Isoamyl Isobutyrate	0.89	0.23	26%	0.90	1%	0.50	0.17	33%	0.31	0.14	44%	0.32	0.45	0.11	0.08	27%	0.18	0.28	0.04	0.05	29%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
NC7-ACET	n-Heptyl Acetate	0.73	0.24	33%	0.74	2%	0.47	0.18	38%	0.27	0.14	53%	0.25	0.41	-0.13	0.12	48%	0.12	0.24	-0.10	0.07	62%
24MC6ACT	2,4-Dimethylhexyl Acetate	0.93	0.29	32%	0.95	2%	0.55	0.20	37%	0.32	0.17	52%	0.30	0.49	-0.12	0.14	45%	0.13	0.28	-0.14	0.09	73%
2ETHXACT	2-Ethyl-Hexyl Acetate	0.79	0.25	32%	0.79	1%	0.49	0.20	40%	0.27	0.16	58%	0.25	0.43	-0.19	0.15	58%	0.10	0.24	-0.18	0.09	97%
34MC6ACT	3,4-Dimethylhexyl Acetate	1.16	0.34	29%	1.18	2%	0.67	0.23	34%	0.41	0.19	45%	0.42	0.60	0.10	0.12	29%	0.22	0.37	0.01	0.07	35%
35MC6ACT	3,5-Dimethylhexyl Acetate	1.09	0.32	29%	1.11	2%	0.62	0.22	35%	0.37	0.18	49%	0.36	0.54	-0.03	0.13	36%	0.18	0.32	-0.07	0.08	47%
3EC6-ACT	3-Ethylhexyl Acetate	1.03	0.31	30%	1.04	2%	0.59	0.21	36%	0.36	0.17	49%	0.35	0.53	-0.01	0.12	35%	0.17	0.31	-0.06	0.08	47%
3MC7-ACT	3-Methylheptyl Aceate	0.76	0.26	34%	0.77	2%	0.47	0.18	39%	0.27	0.15	57%	0.25	0.42	-0.17	0.13	54%	0.10	0.23	-0.16	0.08	87%
45MC6ACT	4,5-Dimethylhexyl Acetate	0.86	0.26	31%	0.87	2%	0.51	0.18	36%	0.30	0.15	49%	0.29	0.45	-0.05	0.11	39%	0.14	0.27	-0.08	0.08	55%
4MC7-ACT	4-Methylheptyl Acetate	0.72	0.24	34%	0.74	2%	0.44	0.17	39%	0.25	0.14	56%	0.23	0.39	-0.14	0.12	52%	0.09	0.21	-0.16	0.08	98%
5MC7-ACT	5-Methylheptyl Aceate	0.73	0.25	34%	0.74	2%	0.46	0.18	39%	0.26	0.15	57%	0.24	0.41	-0.17	0.13	54%	0.09	0.22	-0.16	0.08	89%
NC8-ACET	n-Octyl Acetate	0.64	0.23	36%	0.65	2%	0.41	0.17	41%	0.23	0.14	61%	0.21	0.37	-0.21	0.13	63%	0.07	0.20	-0.17	0.08	112%
235M6ACT	2,3,5-Teimethylhexyl Acetate	0.86	0.28	32%	0.88	2%	0.52	0.20	37%	0.31	0.16	53%	0.29	0.47	-0.12	0.13	46%	0.13	0.28	-0.12	0.09	68%
23MC7ACT	2,3-Dimethylheptyl Acetate	0.84	0.27	33%	0.86	2%	0.51	0.19	38%	0.30	0.16	53%	0.29	0.46	-0.11	0.13	45%	0.12	0.26	-0.12	0.08	69%
24MC7ACT	2,4-Dimethylheptyl Acetate	0.88	0.29	33%	0.90	2%	0.52	0.21	40%	0.29	0.17	59%	0.27	0.47	-0.20	0.15	56%	0.09	0.24	-0.22	0.11	115%
25MC7ACT	2,5-Dimethylheptyl Acetate	0.86	0.28	33%	0.88	2%	0.52	0.20	38%	0.30	0.16	53%	0.29	0.47	-0.13	0.14	47%	0.12	0.27	-0.14	0.09	77%
2MC8-ACT	2-Methyloctyl Acetate	0.63	0.23	37%	0.64	2%	0.40	0.17	43%	0.22	0.14	65%	0.19	0.36	-0.25	0.14	74%	0.05	0.18	-0.23	0.09	189%
35MC7ACT	3,5-Dimethylheptyl Acetate	1.01	0.32	32%	1.03	2%	0.58	0.22	38%	0.34	0.19	55%	0.32	0.53	-0.14	0.15	47%	0.12	0.28	-0.19	0.11	89%
36MC7ACT	3,6-Dimethylheptyl Acetate	0.87	0.29	33%	0.89	2%	0.52	0.20	39%	0.30	0.17	56%	0.28	0.47	-0.17	0.14	52%	0.10	0.25	-0.18	0.10	93%
3EC7-ACT	3-Ethylheptyl Acetate	0.71	0.25	35%	0.72	2%	0.44	0.18	41%	0.24	0.15	61%	0.22	0.40	-0.21	0.14	63%	0.07	0.20	-0.20	0.09	135%
45MC7ACT	4,5-Dimethylheptyl Acetate	0.96	0.30	31%	0.98	2%	0.56	0.21	36%	0.34	0.17	50%	0.33	0.51	-0.05	0.13	39%	0.14	0.29	-0.10	0.09	60%
46MC7ACT	4,6-Dimethylheptyl Acetate	0.83	0.27	33%	0.85	2%	0.48	0.19	39%	0.28	0.16	56%	0.26	0.44	-0.13	0.13	50%	0.10	0.23	-0.18	0.09	99%
4MC8-ACT	4-Methyloctyl Acetate	0.68	0.24	35%	0.70	2%	0.42	0.17	42%	0.23	0.14	61%	0.21	0.38	-0.19	0.13	62%	0.06	0.19	-0.20	0.09	146%
5MC8-ACT	5-Methyloctyl Acetate	0.67	0.24	36%	0.68	2%	0.42	0.17	42%	0.23	0.14	62%	0.21	0.38	-0.22	0.14	65%	0.06	0.20	-0.20	0.09	142%
NC9-ACET	n-Nonyl Acetate	0.58	0.22	38%	0.59	2%	0.38	0.16	43%	0.20	0.14	66%	0.18	0.35	-0.25	0.14	77%	0.04	0.17	-0.22	0.09	198%
36MC8ACT	3,6-Dimethyloctyl Acetate	0.88	0.29	33%	0.89	2%	0.52	0.20	39%	0.30	0.17	55%	0.28	0.47	-0.13	0.14	49%	0.10	0.25	-0.18	0.10	94%
3IPC7ACT	3-Isopropylheptyl Acetate	0.71	0.25	35%	0.73	2%	0.44	0.18	41%	0.25	0.15	59%	0.23	0.40	-0.17	0.13	58%	0.07	0.21	-0.19	0.09	122%
46MC8ACT	4,6-Dimethyloctyl Acetate	0.85	0.29	34%	0.87	2%	0.49	0.20	40%	0.28	0.16	58%	0.27	0.45	-0.15	0.14	54%	0.08	0.23	-0.21	0.10	128%
357M8ACT	3,5,7-Trimethyloctyl Acetate	0.83	0.28	34%	0.85	2%	0.48	0.20	42%	0.27	0.17	62%	0.25	0.44	-0.20	0.15	61%	0.06	0.21	-0.25	0.11	181%
3E6M8ACT	3-Ethyl-6-Methyloctyl Acetate	0.80	0.27	34%	0.82	3%	0.47	0.19	40%	0.27	0.16	58%	0.26	0.44	-0.15	0.14	54%	0.08	0.23	-0.20	0.10	128%
47MC9ACT	4,7-Dimethylnonyl Acetate	0.64	0.24	38%	0.66	3%	0.39	0.17	44%	0.22	0.14	66%	0.19	0.37	-0.22	0.14	72%	0.03	0.17	-0.26	0.10	-
2357M8AC	2,3,5,7-Tetramethyloctyl Acetate	0.74	0.26	36%	0.76	3%	0.44	0.18	42%	0.25	0.15	62%	0.23	0.41	-0.19	0.14	62%	0.05	0.20	-0.23	0.10	190%
357M9ACT	3,5,7-Trimethylnonyl Acetate	0.76	0.27	35%	0.78	2%	0.44	0.19	43%	0.25	0.16	63%	0.23	0.42	-0.20	0.15	64%	0.04	0.19	-0.26	0.11	-
368M9ACT	3,6,8-Trimethylnonyl Acetate	0.72	0.25	35%	0.74	3%	0.42	0.18	42%	0.24	0.15	63%	0.22	0.40	-0.20	0.14	65%	0.05	0.19	-0.24	0.10	-
2468M8AC	2,4,6,8-Tetramethylnonyl Acetate	0.63	0.24	38%	0.64	3%	0.37	0.17	45%	0.21	0.14	69%	0.18	0.36	-0.26	0.14	78%	0.02	0.16	-0.28	0.11	-
3E67M9AC	3-Ethyl-6,7-Dimethylnonyl Acetate	0.76	0.26	34%	0.78	3%	0.45	0.18	40%	0.27	0.15	56%	0.25	0.42	-0.11	0.13	51%	0.07	0.22	-0.18	0.09	129%
479M10AC	4,7,9-Trimethyldecyl Acetate	0.55	0.22	40%	0.57	3%	0.34	0.16	46%	0.19	0.13	71%	0.16	0.32	-0.26	0.13	84%	0.01	0.14	-0.28	0.10	-

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
23568M9A	2,3,5,6,8-Pentaamethylnonyl Acetate	0.74	0.27	36%	0.76	2%	0.45	0.19	42%	0.26	0.16	60%	0.24	0.42	-0.16	0.14	58%	0.06	0.21	-0.22	0.10	182%
3579M10A	3,5,7,9-Tetramethyldecyl Acetate	0.58	0.23	40%	0.60	3%	0.36	0.16	46%	0.20	0.14	70%	0.17	0.35	-0.27	0.14	82%	0.00	0.15	-0.29	0.11	-
5E368M9A	5-Ethyl-3,6,8-Trimethylnonyl Acetate	0.77	0.28	36%	0.79	3%	0.46	0.20	43%	0.27	0.16	61%	0.24	0.44	-0.17	0.15	60%	0.05	0.21	-0.25	0.11	-
DMC	Dimethyl Carbonate	0.06	0.01	21%	0.06	2%	0.04	0.01	20%	0.03	0.01	24%	0.04	0.08	0.01	0.01	37%	0.03	0.05	0.01	0.01	30%
PC	Propylene Carbonate	0.25	0.05	22%	0.26	2%	0.17	0.04	22%	0.13	0.04	27%	0.15	0.29	0.05	0.04	30%	0.10	0.15	0.04	0.02	25%
ME-LACT	Methyl Lactate	2.75	0.58	21%	2.79	1%	1.10	0.30	27%	0.63	0.24	39%	0.73	0.94	0.21	0.12	17%	0.59	0.73	0.38	0.07	11%
MCSVACET	2-Methoxyethyl Acetate	1.18	0.23	19%	1.22	3%	0.64	0.11	17%	0.46	0.11	23%	0.53	0.96	0.25	0.13	25%	0.45	0.70	0.25	0.10	21%
ET-LACT	Ethyl Lactate	2.71	0.59	22%	2.74	1%	1.15	0.31	27%	0.68	0.26	38%	0.79	1.02	0.31	0.12	16%	0.59	0.72	0.38	0.06	11%
MIPR-CB	Methyl Isopropyl Carbonate	0.69	0.13	19%	0.71	2%	0.39	0.07	18%	0.27	0.06	24%	0.32	0.60	0.15	0.08	26%	0.24	0.36	0.14	0.05	20%
PGME-ACT	1-Methoxy-2-Propyl Acetate	1.71	0.31	18%	1.75	3%	0.82	0.15	19%	0.57	0.15	26%	0.66	1.13	0.39	0.14	21%	0.53	0.78	0.38	0.08	15%
CSV-ACET	2-Ethoxyethyl Acetate	1.90	0.34	18%	1.93	2%	0.92	0.18	20%	0.62	0.16	27%	0.71	1.05	0.44	0.12	17%	0.61	0.85	0.43	0.09	14%
2PGMEACT	2-Methyoxy-1-propyl Acetate	1.12	0.20	18%	1.16	4%	0.56	0.09	16%	0.40	0.09	23%	0.46	0.82	0.26	0.10	22%	0.46	0.72	0.27	0.10	21%
DBE-4	Dimethyl Succinate	0.25	0.06	23%	0.25	0%	0.14	0.04	26%	0.10	0.03	33%	0.11	0.16	0.04	0.02	21%	0.07	0.09	0.04	0.01	15%
ETGLDACT	Ethylene Glycol Diacetate	0.72	0.21	29%	0.73	2%	0.42	0.14	34%	0.29	0.12	41%	0.31	0.48	0.12	0.08	27%	0.17	0.23	0.09	0.04	26%
DIPR-CB	Diisopropyl Carbonate	1.04	0.19	19%	1.06	1%	0.54	0.11	20%	0.35	0.09	27%	0.40	0.63	0.23	0.07	18%	0.32	0.42	0.21	0.04	14%
DBE-5	Dimethyl Glutarate	0.49	0.12	24%	0.50	0%	0.28	0.08	29%	0.17	0.06	38%	0.18	0.24	0.08	0.04	20%	0.12	0.16	0.07	0.02	14%
2BUETACT	2-Butoxyethyl Acetate	1.67	0.36	21%	1.70	2%	0.83	0.21	26%	0.56	0.19	33%	0.62	0.82	0.36	0.11	18%	0.44	0.63	0.30	0.07	16%
DBE-6	Dimethyl Adipate	1.95	0.43	22%	1.98	1%	0.91	0.25	28%	0.56	0.21	38%	0.63	0.85	0.43	0.10	16%	0.42	0.50	0.30	0.05	12%
DGEEA	2-(2-Ethoxyethoxy) ethyl acetate	1.50	0.31	21%	1.54	2%	0.76	0.18	24%	0.52	0.16	31%	0.57	0.79	0.31	0.10	17%	0.45	0.69	0.30	0.08	18%
DGBEA	2-(2-Butoxyethoxy) ethyl acetate	1.38	0.32	24%	1.41	2%	0.71	0.20	29%	0.48	0.18	37%	0.52	0.70	0.27	0.10	20%	0.33	0.51	0.11	0.08	24%
SC7ESC12	Substituted C7 ester (C12)	0.92	0.22	24%	0.92	0%	0.48	0.15	32%	0.29	0.12	43%	0.30	0.41	0.08	0.08	25%	0.18	0.27	0.04	0.05	26%
TEXANOL2	1-Hydroxy-2,2,4-Trimethylpentyl-3-Isobutyrate	0.92	0.20	22%	0.93	1%	0.44	0.13	29%	0.26	0.11	40%	0.28	0.37	0.12	0.06	20%	0.18	0.25	0.06	0.04	22%
TEXANOL1	3-Hydroxy-2,2,4-Trimethylpentyl-1-Isobutyrate	0.88	0.23	26%	0.88	0%	0.48	0.16	34%	0.29	0.13	44%	0.30	0.42	0.07	0.08	27%	0.17	0.26	0.02	0.05	28%
TEXANOL	Texanol isomers	0.89	0.22	24%	0.89	0%	0.47	0.15	32%	0.28	0.12	43%	0.30	0.40	0.08	0.07	25%	0.18	0.26	0.04	0.05	26%
SC9ESC12	Substituted C9 Ester (C12)	0.89	0.22	24%	0.89	0%	0.46	0.15	32%	0.28	0.12	43%	0.29	0.40	0.08	0.07	25%	0.18	0.26	0.04	0.05	26%
ETOX	Ethylene Oxide	0.05	0.01	22%	0.05	2%	0.04	0.01	20%	0.03	0.01	25%	0.03	0.07	0.01	0.01	36%	0.02	0.04	0.01	0.01	31%
PROX	Propylene Oxide	0.32	0.07	22%	0.32	1%	0.23	0.05	21%	0.17	0.05	26%	0.20	0.39	0.06	0.06	32%	0.13	0.20	0.05	0.03	27%
12BUOX	1,2-Epoxybutane	1.02	0.25	24%	1.04	2%	0.69	0.17	24%	0.51	0.15	29%	0.58	1.06	0.18	0.16	28%	0.37	0.57	0.16	0.09	24%
FORMACID	Formic Acid	0.08	0.02	21%	0.08	2%	0.05	0.01	20%	0.04	0.01	24%	0.04	0.09	0.01	0.01	34%	0.03	0.05	0.01	0.01	28%
ACETACID	Acetic Acid	0.71	0.13	19%	0.71	1%	0.34	0.07	20%	0.22	0.06	27%	0.26	0.44	0.15	0.05	18%	0.21	0.28	0.14	0.03	13%
ACYRACID	Acrylic Acid	11.66	1.63	14%	11.93	2%	3.99	0.56	14%	2.33	0.53	23%	2.93	4.56	2.34	0.43	15%	3.56	4.45	3.03	0.29	8%
PROPACID	Propionic Acid	1.16	0.25	21%	1.17	1%	0.55	0.14	25%	0.35	0.12	33%	0.40	0.59	0.24	0.06	15%	0.30	0.38	0.22	0.03	10%
ME-ACRYL	Methyl Acrylate	12.24	1.84	15%	12.51	2%	4.21	0.66	16%	2.43	0.60	25%	3.03	4.45	2.50	0.36	12%	3.39	3.90	2.89	0.23	7%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
VIN-ACET	Vinyl Acetate	3.26	0.44	14%	3.35	3%	1.19	0.15	13%	0.73	0.16	21%	0.90	1.39	0.75	0.13	15%	1.07	1.42	0.96	0.11	10%
MBUTENOL	2-Methyl-2-Butene-3-ol	4.12	0.65	16%	5.37	30%	1.65	0.30	18%	1.10	0.28	26%	1.30	2.10	1.07	0.21	16%	1.18	1.53	1.05	0.10	8%
ET-ACRYL	Ethyl Acrylate	8.78	1.37	16%	8.99	2%	3.21	0.55	17%	1.93	0.50	26%	2.36	3.51	2.07	0.24	10%	2.37	2.65	2.18	0.10	4%
ME-MACRT	Methyl Methacrylate	15.84	2.09	13%	16.30	3%	4.95	0.58	12%	2.86	0.60	21%	3.66	6.02	2.61	0.73	20%	4.89	6.11	3.96	0.50	10%
BU-MACRT	Butyl Methacrylate	9.09	1.21	13%	9.37	3%	2.91	0.35	12%	1.67	0.36	22%	2.11	3.20	1.59	0.36	17%	2.69	3.32	2.22	0.25	9%
IBUMACRT	Isobutyl Methacrylate	8.99	1.19	13%	9.26	3%	2.87	0.34	12%	1.63	0.35	22%	2.07	3.15	1.54	0.37	18%	2.67	3.29	2.20	0.26	10%
FURAN	Furan	16.54	2.32	14%	16.98	3%	4.97	0.73	15%	2.41	0.74	31%	3.05	5.13	0.83	0.79	26%	4.49	5.29	3.51	0.42	9%
FORMALD	Formaldehyde	8.97	1.32	15%	9.24	3%	2.56	0.32	12%	1.27	0.31	24%	1.71	3.51	0.88	0.56	33%	2.95	4.18	2.08	0.48	16%
ACETALD	Acetaldehyde	6.84	1.14	17%	7.06	3%	2.56	0.44	17%	1.70	0.42	25%	2.09	3.83	1.64	0.42	20%	1.79	2.16	1.42	0.17	9%
PROPALD	Propionaldehyde	7.89	1.43	18%	8.13	3%	2.97	0.59	20%	1.95	0.55	28%	2.37	4.02	1.84	0.43	18%	2.00	2.60	1.60	0.21	11%
2MEC3AL	2-Methylpropanal	5.87	1.05	18%	6.07	3%	2.25	0.43	19%	1.51	0.41	27%	1.83	3.22	1.40	0.36	20%	1.57	1.92	1.24	0.16	10%
1C4RCHO	Butanal	6.74	1.22	18%	6.92	3%	2.55	0.52	20%	1.67	0.47	28%	2.03	3.41	1.57	0.37	18%	1.70	2.20	1.36	0.18	11%
C4-RCHO	C4 aldehydes	6.74	1.22	18%	6.92	3%	2.55	0.52	20%	1.67	0.47	28%	2.03	3.41	1.57	0.37	18%	1.70	2.20	1.36	0.18	11%
22DMC3AL	2,2-Dimethylpropanal (pivaldehyde)	5.40	0.96	18%	5.57	3%	2.03	0.39	19%	1.35	0.37	27%	1.64	2.87	1.26	0.32	19%	1.41	1.80	1.12	0.15	10%
3MC4RCHO	3-Methylbutanal (Isovaleraldehyde)	5.52	0.96	17%	5.68	3%	2.08	0.39	19%	1.37	0.37	27%	1.66	2.79	1.30	0.30	18%	1.46	1.82	1.17	0.14	10%
1C5RCHO	Pentanal (Valeraldehyde)	5.76	1.04	18%	5.94	3%	2.20	0.44	20%	1.45	0.40	28%	1.76	2.98	1.35	0.33	19%	1.47	1.86	1.15	0.16	11%
C5-RCHO	C5 Aldehydes	5.76	1.04	18%	5.94	3%	2.20	0.44	20%	1.45	0.40	28%	1.76	2.98	1.35	0.33	19%	1.47	1.86	1.15	0.16	11%
GLTRALD	Glutaraldehyde	4.79	0.89	19%	4.96	3%	1.84	0.36	19%	1.25	0.34	27%	1.52	2.74	1.12	0.33	22%	1.27	1.55	0.92	0.15	12%
1C6RCHO	Hexanal	4.98	0.89	18%	5.12	3%	1.89	0.38	20%	1.23	0.35	28%	1.48	2.44	1.17	0.25	17%	1.25	1.61	1.01	0.13	10%
C6-RCHO	C6 Aldehydes	4.98	0.89	18%	5.12	3%	1.89	0.38	20%	1.23	0.35	28%	1.48	2.44	1.17	0.25	17%	1.25	1.61	1.01	0.13	10%
1C7RCHO	Heptanal	4.23	0.76	18%	4.36	3%	1.61	0.33	21%	1.04	0.30	29%	1.26	1.97	0.98	0.20	16%	1.05	1.35	0.82	0.11	11%
C7-RCHO	C7 Aldehydes	4.23	0.76	18%	4.36	3%	1.61	0.33	21%	1.04	0.30	29%	1.26	1.97	0.98	0.20	16%	1.05	1.35	0.82	0.11	11%
1C8RCHO	Octanal	3.65	0.67	18%	3.74	3%	1.40	0.30	21%	0.90	0.27	29%	1.08	1.64	0.83	0.17	15%	0.89	1.15	0.65	0.10	11%
C8-RCHO	C8 Aldehydes	3.65	0.67	18%	3.74	3%	1.40	0.30	21%	0.90	0.27	29%	1.08	1.64	0.83	0.17	15%	0.89	1.15	0.65	0.10	11%
GLYOXAL	Glyoxal	14.22	2.15	15%	14.72	3%	4.05	0.54	13%	2.02	0.51	25%	2.72	5.26	1.33	0.94	35%	5.19	7.64	3.30	0.91	17%
MEGLYOX	Methyl Glyoxal	16.21	2.37	15%	16.82	4%	4.67	0.54	12%	2.49	0.56	23%	3.31	5.95	1.92	0.94	28%	5.63	7.77	4.00	0.88	16%
ACROLEIN	Acrolein	7.60	1.43	19%	7.78	2%	2.78	0.60	22%	1.80	0.55	31%	2.19	3.61	1.60	0.41	19%	1.71	2.12	1.23	0.24	14%
CROTALD	Crotonaldehyde	10.07	1.52	15%	10.33	3%	3.50	0.54	15%	2.13	0.51	24%	2.67	4.40	2.14	0.40	15%	2.75	3.25	2.29	0.19	7%
METHACRO	Methacrolein	6.23	1.02	16%	6.41	3%	2.24	0.40	18%	1.42	0.37	26%	1.75	2.94	1.38	0.30	17%	1.62	1.92	1.26	0.15	9%
HOMACR	Hydroxy Methacrolein	6.61	1.06	16%	6.78	3%	2.37	0.41	17%	1.46	0.38	26%	1.81	2.90	1.49	0.26	14%	1.76	1.98	1.46	0.11	6%
BENZALD	Benzaldehyde	-0.61	0.23	-37%	-0.60	-1%	-1.64	0.24	-15%	-2.32	0.66	-29%	-2.79	-0.32	-11.54	2.06	-74%	-1.67	-0.44	-4.95	1.05	-63%
TOLUALD	Tolualdehyde	-0.54	0.20	-37%	-0.53	-1%	-1.45	0.22	-15%	-2.05	0.59	-29%	-2.47	-0.28	-10.19	1.82	-74%	-1.47	-0.38	-4.37	0.93	-63%
ACETONE	Acetone	0.43	0.08	19%	0.43	2%	0.17	0.04	21%	0.11	0.03	29%	0.13	0.19	0.10	0.02	13%	0.10	0.13	0.08	0.01	9%
CC4-KET	Cyclobutanone	0.68	0.18	26%	0.69	1%	0.41	0.12	30%	0.29	0.11	37%	0.31	0.48	0.12	0.08	24%	0.19	0.27	0.11	0.04	19%
MEK	Methyl Ethyl Ketone	1.49	0.31	21%	1.52	2%	0.66	0.18	26%	0.43	0.15	35%	0.49	0.72	0.35	0.08	16%	0.34	0.44	0.28	0.03	10%
CC5-KET	Cyclopentanone	1.43	0.37	26%	1.44	1%	0.84	0.25	30%	0.59	0.22	37%	0.65	0.96	0.25	0.16	24%	0.39	0.54	0.22	0.08	20%
KET5C	C5 Cyclic Ketones	1.43	0.37	26%	1.44	1%	0.84	0.25	30%	0.59	0.22	37%	0.65	0.96	0.25	0.16	24%	0.39	0.54	0.22	0.08	20%
MPK	2-Pentanone	3.07	0.65	21%	3.12	2%	1.50	0.37	25%	1.01	0.32	31%	1.16	1.87	0.71	0.22	19%	0.80	1.06	0.64	0.10	12%
DEK	3-Pentanone	1.45	0.36	25%	1.46	1%	0.73	0.24	32%	0.49	0.20	41%	0.54	0.80	0.32	0.13	24%	0.32	0.45	0.21	0.06	18%
KET5	C5 Ketones	3.07	0.65	21%	3.12	2%	1.50	0.37	25%	1.01	0.32	31%	1.16	1.87	0.71	0.22	19%	0.80	1.06	0.64	0.10	12%
CC6-KET	Cyclohexanone	1.61	0.43	26%	1.62	1%	0.90	0.29	32%	0.61	0.24	40%	0.65	0.94	0.28	0.15	23%	0.36	0.52	0.22	0.08	23%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
KET6C	C6 Cyclic Ketones	1.61	0.43	26%	1.62	1%	0.90	0.29	32%	0.61	0.24	40%	0.65	0.94	0.28	0.15	23%	0.36	0.52	0.22	0.08	23%
MIBK	4-Methyl-2-Pentanone	4.31	0.73	17%	4.40	2%	1.83	0.32	17%	1.21	0.30	25%	1.45	2.49	1.13	0.25	18%	1.21	1.58	1.07	0.11	9%
MNBK	Methyl n-Butyl Ketone	3.55	0.76	21%	3.62	2%	1.71	0.43	25%	1.15	0.37	32%	1.32	2.00	0.80	0.25	19%	0.90	1.17	0.73	0.11	13%
MTBK	Methyl t-Butyl Ketone	0.78	0.17	21%	0.80	2%	0.39	0.09	24%	0.26	0.08	31%	0.29	0.44	0.19	0.04	15%	0.20	0.25	0.17	0.02	9%
KET6	C6 Ketones	3.55	0.76	21%	3.62	2%	1.71	0.43	25%	1.15	0.37	32%	1.32	2.00	0.80	0.25	19%	0.90	1.17	0.73	0.11	13%
KET7C	C7 Cyclic Ketones	1.41	0.37	26%	1.42	1%	0.79	0.25	32%	0.53	0.21	40%	0.57	0.82	0.24	0.13	23%	0.32	0.46	0.19	0.07	23%
C7-KET-2	2-Heptanone	2.80	0.64	23%	2.85	2%	1.40	0.39	28%	0.93	0.33	36%	1.03	1.41	0.58	0.19	18%	0.66	0.85	0.47	0.10	15%
2M-3-HXO	2-Methyl-3-Hexanone	1.79	0.44	24%	1.82	2%	0.94	0.28	30%	0.62	0.24	38%	0.69	0.97	0.35	0.15	21%	0.41	0.54	0.25	0.08	19%
DIPK	Di-Isopropyl Ketone	1.63	0.41	25%	1.65	1%	0.87	0.28	32%	0.58	0.23	40%	0.63	0.91	0.30	0.14	23%	0.36	0.48	0.20	0.08	22%
KET7	C7 Ketones	2.80	0.64	23%	2.85	2%	1.40	0.39	28%	0.93	0.33	36%	1.03	1.41	0.58	0.19	18%	0.66	0.85	0.47	0.10	15%
KET8C	C8 Cyclic Ketones	1.25	0.33	26%	1.26	1%	0.70	0.22	32%	0.47	0.19	40%	0.51	0.73	0.21	0.12	23%	0.28	0.41	0.17	0.06	23%
C8-KET-2	2-Octanone	1.66	0.43	26%	1.68	1%	0.92	0.29	32%	0.58	0.24	41%	0.61	0.81	0.29	0.14	23%	0.35	0.52	0.12	0.09	25%
KET8	C8 Ketones	1.66	0.43	26%	1.68	1%	0.92	0.29	32%	0.58	0.24	41%	0.61	0.81	0.29	0.14	23%	0.35	0.52	0.12	0.09	25%
KET9C	C9 Cyclic Ketones	1.13	0.30	26%	1.13	1%	0.63	0.20	32%	0.42	0.17	40%	0.46	0.66	0.19	0.11	23%	0.26	0.37	0.15	0.06	23%
C9-KET-2	2-Nonanone	1.30	0.36	28%	1.32	1%	0.74	0.26	35%	0.45	0.22	48%	0.45	0.67	0.04	0.15	34%	0.22	0.40	-0.06	0.10	45%
DIBK	Di-isobutyl ketone (2,6-dimethyl-4-heptanone)	2.94	0.59	20%	3.00	2%	1.29	0.31	24%	0.85	0.28	33%	0.97	1.31	0.69	0.16	16%	0.65	0.85	0.31	0.11	17%
KET9	C9 Ketones	1.30	0.36	28%	1.32	1%	0.74	0.26	35%	0.45	0.22	48%	0.45	0.67	0.04	0.15	34%	0.22	0.40	-0.06	0.10	45%
KET10C	C10 Cyclic Ketones	1.02	0.27	26%	1.03	1%	0.57	0.18	32%	0.39	0.15	40%	0.42	0.60	0.18	0.10	23%	0.23	0.33	0.14	0.05	23%
C10-K-2	2-Decanone	1.06	0.33	31%	1.07	1%	0.62	0.24	39%	0.36	0.20	55%	0.34	0.57	-0.12	0.16	47%	0.14	0.31	-0.18	0.11	82%
KET10	C10 Ketones	1.06	0.33	31%	1.07	1%	0.62	0.24	39%	0.36	0.20	55%	0.34	0.57	-0.12	0.16	47%	0.14	0.31	-0.18	0.11	82%
BIACETYL	Biacetyl	20.73	3.02	15%	21.50	4%	6.09	0.69	11%	3.38	0.75	22%	4.44	7.37	2.68	1.17	26%	7.45	10.51	5.49	1.14	15%
MVK	Methylvinyl ketone	8.73	1.34	15%	8.96	3%	3.31	0.55	17%	2.11	0.52	25%	2.59	4.39	2.17	0.40	15%	2.35	2.70	2.10	0.14	6%
HOACET	Hydroxy Acetone	3.08	0.54	18%	3.15	2%	1.13	0.23	20%	0.66	0.19	30%	0.80	1.12	0.61	0.08	10%	0.70	0.82	0.60	0.05	7%
MEOACET	Methoxy Acetone	2.14	0.43	20%	2.18	2%	1.01	0.21	21%	0.70	0.19	28%	0.82	1.45	0.52	0.17	21%	0.60	0.82	0.49	0.08	13%
DIACTALC	Diacetone Alcohol	0.68	0.16	24%	0.69	1%	0.36	0.11	31%	0.23	0.09	39%	0.26	0.36	0.14	0.05	20%	0.16	0.21	0.11	0.02	14%
PHENOL	Phenol	1.82	0.28	15%	1.88	3%	-0.74	0.28	-38%	-1.67	0.65	-39%	-1.99	0.37	-11.6	2.09	-105%	-0.72	0.32	-4.54	0.99	-137%
CRESOL	Alkyl Phenols	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
M-CRESOL	m-Cresol	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
P-CRESOL	p-Cresol	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
O-CRESOL	o-Cresol	2.34	0.34	15%	2.42	3%	-0.72	0.24	-33%	-1.81	0.65	-36%	-2.14	0.57	-12.1	2.24	-105%	-0.76	0.52	-4.83	1.17	-153%
NO2-BENZ	Nitrobenzene	0.07	0.02	24%	0.07	0%	0.03	0.01	40%	0.01	0.01	77%	0.01	0.02	-0.03	0.01	65%	0.01	0.02	0.00	0.00	21%
P-TI	Para Toluene Isocyanate	0.93	0.20	21%	0.95	2%	-0.85	0.33	-39%	-1.44	0.61	-42%	-1.69	0.16	-9.22	1.63	-97%	-0.58	0.13	-3.01	0.60	-104%
TDI	Toluene Diisocyanate	-0.13	0.07	-55%	-0.13	1%	-1.02	0.26	-25%	-1.38	0.51	-37%	-1.63	-0.10	-8.19	1.39	-86%	-0.77	-0.13	-2.98	0.53	-69%
MDI	Methylene Diphenylene Diisocyanate	0.79	0.15	19%	0.81	3%	-0.48	0.21	-44%	-0.91	0.40	-44%	-1.07	0.15	-6.35	1.12	-104%	-0.38	0.13	-2.20	0.44	-118%
DM-AMINE	Dimethyl Amine	9.37	1.48	16%	9.69	3%	3.60	0.56	16%	2.36	0.56	24%	2.88	4.78	2.39	0.48	17%	3.03	3.85	2.68	0.29	10%
ET-AMINE	Ethyl Amine	7.80	1.29	17%	8.01	3%	3.20	0.55	17%	2.14	0.53	25%	2.57	4.34	2.07	0.44	17%	2.42	3.16	2.12	0.26	11%
TM-AMINE	Trimethyl Amine	7.06	1.11	16%	7.31	3%	2.73	0.43	16%	1.79	0.42	24%	2.18	3.64	1.82	0.36	17%	2.27	2.90	2.01	0.22	10%
ETOH-NH2	Ethanolamine	5.97	0.98	16%	6.15	3%	2.42	0.41	17%	1.62	0.39	24%	1.94	3.28	1.57	0.33	17%	1.86	2.43	1.64	0.20	11%
DMAE	Dimethylaminoethanol	4.76	0.76	16%	4.93	4%	1.81	0.29	16%	1.17	0.29	25%	1.42	2.24	1.20	0.21	15%	1.48	1.84	1.34	0.12	8%
ETOH2-NH	Diethanol Amine	4.05	0.65	16%	4.20	4%	1.54	0.25	16%	1.00	0.24	24%	1.21	1.90	1.02	0.18	15%	1.26	1.57	1.14	0.10	8%
ETOH3-N	Triethanolamine	2.76	0.46	17%	2.86	4%	1.05	0.19	18%	0.67	0.18	26%	0.81	1.17	0.69	0.11	13%	0.80	0.99	0.62	0.06	8%
NMP	N-Methyl-2-Pyrrolidone	2.56	0.59	23%	2.59	1%	1.23	0.36	29%	0.80	0.31	39%	0.89	1.24	0.56	0.17	19%	0.56	0.71	0.37	0.08	15%
CH3-CL	Methyl Chloride	0.03	0.01	24%	0.03	1%	0.02	0.01	27%	0.01	0.00	33%	0.02	0.03	0.01	0.00	25%	0.01	0.02	0.01	0.00	19%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
CL-ETHE	Vinyl Chloride	2.92	0.59	20%	2.98	2%	1.43	0.31	21%	0.98	0.27	28%	1.14	1.96	0.66	0.23	20%	0.87	1.17	0.62	0.13	14%
C2-CL	Ethyl Chloride	0.25	0.06	24%	0.25	1%	0.14	0.04	27%	0.10	0.03	33%	0.11	0.19	0.05	0.03	24%	0.07	0.11	0.04	0.01	18%
CL2-ME	Dichloromethane	0.07	0.02	24%	0.07	1%	0.04	0.01	27%	0.03	0.01	33%	0.03	0.05	0.01	0.01	24%	0.02	0.03	0.01	0.00	19%
ME-BR	Methyl Bromide	0.02	0.00	24%	0.02	1%	0.01	0.00	27%	0.01	0.00	33%	0.01	0.01	0.00	0.00	25%	0.01	0.01	0.00	0.00	19%
11CL2-C2	1,1-Dichloroethane	0.10	0.02	24%	0.10	1%	0.06	0.02	27%	0.04	0.01	33%	0.05	0.08	0.02	0.01	24%	0.03	0.04	0.02	0.01	18%
12CL2-C2	1,2-Dichloroethane	0.10	0.02	24%	0.10	1%	0.06	0.02	27%	0.04	0.01	33%	0.05	0.08	0.02	0.01	24%	0.03	0.04	0.02	0.01	18%
C2-BR	Ethyl Bromide	0.11	0.03	24%	0.11	1%	0.06	0.02	27%	0.04	0.01	33%	0.05	0.08	0.02	0.01	24%	0.03	0.05	0.02	0.01	18%
CHCL3	Chloroform	0.03	0.01	24%	0.03	1%	0.02	0.01	27%	0.01	0.00	33%	0.02	0.03	0.01	0.00	25%	0.01	0.02	0.01	0.00	19%
C3-BR	n-Propyl Bromide	0.35	0.08	23%	0.35	1%	0.20	0.05	26%	0.14	0.04	32%	0.16	0.26	0.07	0.04	23%	0.10	0.15	0.06	0.02	18%
111-TCE	1,1,1-Trichloroethane	0.00	0.00	24%	0.00	1%	0.00	0.00	27%	0.00	0.00	33%	0.00	0.00	0.00	0.00	25%	0.00	0.00	0.00	0.00	19%
112CL3C2	1,1,2-Trichloroethane	0.06	0.01	24%	0.06	1%	0.03	0.01	27%	0.02	0.01	33%	0.03	0.05	0.01	0.01	24%	0.02	0.03	0.01	0.00	19%
C4-BR	n-Butyl Bromide	0.60	0.13	22%	0.61	1%	0.33	0.08	24%	0.23	0.07	31%	0.26	0.44	0.12	0.06	22%	0.18	0.25	0.11	0.03	17%
11BR2-C2	1,2-Dibromoethane	0.05	0.01	24%	0.05	1%	0.03	0.01	27%	0.02	0.01	33%	0.02	0.04	0.01	0.01	24%	0.01	0.02	0.01	0.00	18%
T-12-DCE	Trans-1,2-Dichloroethene	0.81	0.18	22%	0.82	1%	0.44	0.11	25%	0.31	0.10	31%	0.35	0.60	0.16	0.08	22%	0.24	0.34	0.15	0.04	17%
CL2IBUTE	2-(Cl-methyl)-3-Cl-Propene	1.13	0.31	28%	1.18	4%	0.61	0.17	29%	0.47	0.15	32%	0.53	0.94	0.27	0.18	33%	0.22	0.70	-0.15	0.13	61%
CL3-ETHE	Trichloroethylene	0.60	0.13	22%	0.61	1%	0.33	0.08	25%	0.23	0.07	31%	0.26	0.44	0.12	0.06	22%	0.18	0.25	0.11	0.03	17%
CL4-ETHE	Perchloroethylene	0.04	0.01	24%	0.04	1%	0.02	0.01	27%	0.02	0.01	33%	0.02	0.03	0.01	0.00	24%	0.01	0.02	0.01	0.00	18%
CL-BEN	Monochlorobenzene	0.36	0.09	24%	0.36	0%	0.15	0.06	39%	0.07	0.05	75%	0.08	0.13	-0.14	0.05	64%	0.08	0.10	0.02	0.02	20%
CF3-BEN	Benzotrifluoride	0.26	0.06	21%	0.27	1%	0.08	0.03	36%	0.02	0.03	131%	0.02	0.08	-0.15	0.04	173%	0.05	0.07	0.00	0.01	29%
CL2-BEN	p-Dichlorobenzene	0.20	0.05	24%	0.20	1%	0.09	0.03	39%	0.04	0.03	76%	0.04	0.07	-0.08	0.03	64%	0.04	0.05	0.01	0.01	20%
PCBTF	p-Trifluoromethyl-Cl-Benzene	0.11	0.02	21%	0.11	1%	0.04	0.01	36%	0.01	0.01	133%	0.01	0.03	-0.07	0.02	176%	0.02	0.03	0.00	0.01	29%
Mixtures																						
ARBROG	Base ROG Mixture	3.71	0.63	17%	3.79	2%	1.46	0.28	19%	0.85	0.25	30%	1.00	1.00	1.00			1.00	1.00	1.00		
RFA-TLEV	TLEV Exhaust -- RFA	4.09	0.68	17%	4.21	3%	1.58	0.30	19%	0.89	0.27	30%	1.06	1.12	0.93	0.04	4%	1.10	1.15	1.06	0.02	2%
PH2-TLEV	TLEV Exhaust -- Phase 2	4.05	0.66	16%	4.15	2%	1.57	0.29	18%	0.90	0.26	29%	1.07	1.12	1.01	0.03	3%	1.11	1.16	1.08	0.02	2%
LPG-TLEV	TLEV Exhaust -- LPG	2.11	0.35	16%	2.15	2%	0.91	0.15	17%	0.58	0.15	25%	0.69	1.11	0.57	0.10	14%	0.64	0.83	0.58	0.06	9%
CNG-TLEV	TLEV Exhaust -- CNG	0.75	0.13	18%	0.76	2%	0.35	0.07	20%	0.23	0.06	28%	0.27	0.44	0.20	0.04	16%	0.23	0.30	0.21	0.02	10%
E85-TLEV	TLEV Exhaust -- E-85	2.70	0.53	20%	2.75	2%	1.24	0.28	23%	0.82	0.25	30%	0.96	1.51	0.66	0.16	16%	0.74	0.94	0.64	0.07	9%
M85-TLEV	TLEV Exhaust -- M-85	1.57	0.24	16%	1.61	2%	0.61	0.09	15%	0.35	0.09	25%	0.43	0.60	0.35	0.05	12%	0.47	0.60	0.41	0.04	8%
RFA-LEV	Final LEV -- RFA	3.64	0.62	17%	3.73	2%	1.43	0.28	20%	0.81	0.25	31%	0.95	1.00	0.77	0.04	4%	0.96	1.01	0.92	0.02	2%
PH2-LEV	Final LEV -- Phase 2	3.55	0.60	17%	3.65	3%	1.42	0.27	19%	0.82	0.24	30%	0.96	1.01	0.92	0.02	2%	0.97	1.02	0.92	0.02	2%
MS-D	Mineral Spirits "D" (Type II-C)	0.79	0.30	38%	0.81	3%	0.48	0.22	45%	0.27	0.18	68%	0.23	0.46	-0.32	0.18	78%	0.03	0.21	-0.34	0.13	-
MS-A	Mineral Spirits "A" (Type I-B, 91% Alkanes)	1.27	0.36	28%	1.30	2%	0.65	0.24	36%	0.36	0.20	54%	0.35	0.56	-0.20	0.17	49%	0.17	0.33	-0.17	0.12	73%
MS-B	Mineral Spirits "B" (Type II-C)	0.78	0.30	38%	0.80	3%	0.48	0.21	45%	0.26	0.18	68%	0.23	0.45	-0.31	0.18	77%	0.03	0.21	-0.34	0.13	-
MS-C	Mineral Spirits "C" (Type II-C)	0.78	0.30	38%	0.80	3%	0.48	0.21	45%	0.26	0.18	68%	0.23	0.45	-0.32	0.18	79%	0.03	0.21	-0.34	0.13	-
D95	Exxon Exxol(r) D95 Fluid	0.67	0.27	40%	0.68	2%	0.42	0.19	47%	0.23	0.16	71%	0.20	0.40	-0.32	0.17	84%	0.01	0.18	-0.33	0.12	-
ISOPARM	Exxon Isopar(r) M Fluid	0.65	0.26	40%	0.67	3%	0.41	0.19	46%	0.23	0.16	71%	0.19	0.39	-0.31	0.16	84%	0.01	0.18	-0.32	0.12	-
OC6-ACET	Oxo-Hexyl Acetate	1.03	0.29	28%	1.04	2%	0.61	0.20	33%	0.38	0.16	42%	0.39	0.54	0.13	0.10	26%	0.22	0.35	0.07	0.06	25%
OC7-ACET	Oxo-Heptyl Acetate	0.97	0.29	29%	0.99	2%	0.57	0.20	34%	0.35	0.16	46%	0.35	0.50	0.02	0.11	32%	0.18	0.31	-0.02	0.07	38%

Table C-6 (continued)

Name	Compound or Mixture	MIR (gm O3 / gm VOC)					MOIR (gm/gm)			EBIR (gm/gm)			Base Case Relative Reactivities [a]								
		39 Scenarios			Avg. Conds		39 Scenarios			39 Scenarios			Ozone Yield (gm basis)					Max 8-Hour Avg (gm basis)				
		Avg.	Sdev			Δ%	Avg.	Sdev		Avg.	Sdev		Avg.	Max	Min	Sdev		Avg.	Max	Min	Sdev	
OC8-ACET	Oxo-Octyl Acetate	0.96	0.29	31%	0.98	2%	0.56	0.20	36%	0.33	0.16	50%	0.33	0.50	-0.05	0.12	38%	0.15	0.29	-0.09	0.08	53%
OC9-ACET	Oxo-Nonyl Acetate	0.85	0.28	33%	0.87	2%	0.50	0.20	39%	0.29	0.16	56%	0.27	0.46	-0.15	0.14	51%	0.10	0.25	-0.18	0.10	95%
OC10ACET	Oxo-Decyl Acetate	0.83	0.28	33%	0.85	2%	0.49	0.19	40%	0.28	0.16	57%	0.27	0.45	-0.15	0.14	52%	0.09	0.24	-0.19	0.10	108%
OC12ACET	Oxo-Dodecyl Acetate	0.72	0.26	36%	0.74	2%	0.43	0.18	42%	0.24	0.15	63%	0.22	0.40	-0.19	0.14	64%	0.05	0.19	-0.24	0.11	-
OC13ACET	Oxo-Tridecyl Acetate	0.67	0.25	37%	0.69	3%	0.40	0.17	43%	0.23	0.15	64%	0.21	0.38	-0.20	0.14	66%	0.04	0.18	-0.25	0.10	-

[a] Maximum, minimum, and standard deviations for base ROG mixture are incremental reactivities relative to the average.

Table C-7. Ozone yield incremental reactivities in the individual base case and adjusted NO_x scenarios. (This table is included with the electronic version of the report only.)

Table C-8. Maximum 8-hour average incremental reactivities in the individual base case and adjusted NO_x scenarios. (This table is included with the electronic version of the report only.)