APPENDIX A.

MECHANISM LISTING AND TABULATIONS

This Appendix contains the tables giving a complete listing of the both the detailed and the condensed versions of the SAPRC-99 mechanism. Table A-1 contains a list of all the model species used in both versions. Table A-2 lists all the reactions and rate parameters in the base mechanism, and Table A-3 gives the additional reactions and rate parameters used in the fixed parameter version of the lumped mechanism. Both tables have footnotes documenting the rate parameters and reactions used, and the text of these footnotes are given in Table A-4. Table A-5 lists the absorption cross sections and photolysis reactions used in the mechanism. Finally, Table A-6 lists the reactions and rate parameters derived or assigned to all the VOCs that are not incorporated in the base or condensed mechanisms. These are added to the base mechanism as needed to evaluate the mechanism for the individual VOC, or to assess its atmospheric reactivity. Note that the reactions of the VOCs that are explicitly represented in the condensed mechanism, such as ethylene and isoprene, are given in Table A-2 rather than Table A-6.

Table A-1. Listing of model species used in the base and lumped mechanisms.

Type and Name	Description
	Species used in Base Mechanism
Constant Species.	
O2	Oxygen
M	Air
H2O	Water
H2	Hydrogen Molecules
HV	Light
Active Inorganic Species.	
O3	Ozone
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
N2O5	Nitrogen Pentoxide
HONO	Nitrous Acid
HNO3	Nitric Acid
HNO4	Peroxynitric Acid
HO2H	Hydrogen Peroxide
CO	Carbon Monoxide
SO2	Sulfur Dioxide
Active Radical Species and Operators.	
HO.	Hydroxyl Radicals
HO2.	Hydroperoxide Radicals
C-O2.	Methyl Peroxy Radicals
RO2-R.	Peroxy Radical Operator representing NO to NO2 conversion with HO2 formation.
R2O2.	Peroxy Radical Operator representing NO to NO2 conversion without HO2 formation.
RO2-N.	Peroxy Radical Operator representing NO consumption with organic nitrate formation.
CCO-O2.	Acetyl Peroxy Radicals
RCO-O2.	Peroxy Propionyl and higher peroxy acyl Radicals
BZCO-O2.	Peroxyacyl radical formed from Aromatic Aldehydes
MA-RCO3.	Peroxyacyl radicals formed from methacrolein and other acroleins.
Steady State Radical Species	
O3P	Ground State Oxygen Atoms
O*1D2	Excited Oxygen Atoms
TBU-O.	t-Butoxy Radicals
BZ-O.	Phenoxy Radicals
BZ(NO2)-O.	Nitro-substituted Phenoxy Radical
HOCOO.	Radical formed when Formaldehyde reacts with HO2
PAN and PAN Analogues	
PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues
PBZN	PAN analogues formed from Aromatic Aldehydes
MA-PAN	PAN analogue formed from Methacrolein

Table A-1 (continued)

Type and Name	Description
Explicit and Lumped Molecule Reactive Organic Product Species	
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals slower than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
MEOH	Methanol
COOH	Methyl Hydroperoxide
ROOH	Lumped higher organic hydroperoxides
GLY	Glyoxal
MGLY	Methyl Glyoxal
BACL	Biacetyl
PHEN	Phenol
CRES	Cresols
NPHE	Nitrophenols
BALD	Aromatic aldehydes (e.g., benzaldehyde)
METHACRO	Methacrolein
MVK	Methyl Vinyl Ketone
ISO-PROD	Lumped isoprene product species
Lumped Parameter Products	
PROD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5 x 10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
RNO3	Lumped Organic Nitrates
Uncharacterized Reactive Aromatic Ring Fragmentation Products	
DCB1	Reactive Aromatic Fragmentation Products that do not undergo signficant photodecomposition to radicals.
DCB2	Reactive Aromatic Fragmentation Products which photolyze with alpha-dicarbonyl-like action spectrum.
DCB3	Reactive Aromatic Fragmentation Products which photolyze with acrolein action spectrum.
Non-Reacting Species	
CO2	Carbon Dioxide
XC	Lost Carbon
XN	Lost Nitrogen
SULF	Sulfates (SO_3 or H_2SO_4)
Low Reactivity Compounds or Unknown Products Represented as Unreactive	
H2	Hydrogen
HCOOH	Formic Acid
CCO-OH	Acetic Acid
RCO-OH	Higher organic acids
CCO-OOH	Peroxy Acetic Acid
RCO-OOH	Higher organic peroxy acids
NROG	Unspecified Unreactive Carbon

Table A-1 (continued)

Type and Name	Description
	Species used in Lumped Mechanisms for Base Case and Ambient Simulations
Primary Organics Represented explicitly	
CH4	Methane
ETHENE	Ethene
ISOPRENE	Isoprene
Lumped Parameter Species	
ALK1	Alkanes and other non-aromatic compounds that react only with OH, and have kOH < 5 x 10^2 ppm-1 min-1. (Primarily ethane)
ALK2	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^2 and 2.5 x 10^3 ppm-1 min-1. (Primarily propane and acetylene)
ALK3	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 2.5 x 10^3 and 5 x 10^3 ppm-1 min-1.
ALK4	Alkanes and other non-aromatic compounds that react only with OH, and have kOH between 5 x 10^3 and 1 x 10^4 ppm-1 min-1.
ALK5	Alkanes and other non-aromatic compounds that react only with OH, and have kOH greater than 1 x 10^4 ppm-1 min-1.
ARO1	Aromatics with kOH < 2x10^4 ppm-1 min-1.
ARO2	Aromatics with kOH > 2x10^4 ppm-1 min-1.
OLE1	Alkenes (other than ethene) with kOH < 7x10^4 ppm-1 min-1.
OLE2	Alkenes with kOH > 7x10^4 ppm-1 min-1.
TERP	Terpenes

Table A-2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
Inorganic Reactions						
1		Phot Set= NO2			1,2	NO2 + HV = NO + O3P
2	5.79e-34	5.68e-34	0.00	-2.8	3	O3P + O2 + M = O3 + M
3	7.96e-15	8.00e-12	4.09		4,5	O3P + O3 = #2 O2
4	1.01e-31	1.00e-31	0.00	-1.6	6,7,5	O3P + NO + M = NO2 + M
5	9.72e-12	6.50e-12	-0.24		4,5	O3P + NO2 = NO + O2
6	1.82e-12	Falloff, F=0.80			4,7,5,8	O3P + NO2 = NO3 + M
	0:	9.00e-32	0.00	-2.0		
	inf:	2.20e-11	0.00	0.0		
8	1.81e-14	1.80e-12	2.72		6	O3 + NO = NO2 + O2
9	3.52e-17	1.40e-13	4.91		6	O3 + NO2 = O2 + NO3
10	2.60e-11	1.80e-11	-0.22		6	NO + NO3 = #2 NO2
11	1.95e-38	3.30e-39	-1.05		6	NO + NO + O2 = #2 NO2
12	1.54e-12	Falloff, F=0.45			6,7	NO2 + NO3 = N2O5
	0:	2.80e-30	0.00	-3.5		
	inf:	2.00e-12	0.00	0.2		
13	5.28e-2	Falloff, F=0.45			6,7	N2O5 = NO2 + NO3
	0:	1.00e-3	21.86	-3.5		
	inf:	9.70e+14	22.02	0.1		
14	2.60e-22	2.60e-22			9	N2O5 + H2O = #2 HNO3
15		(Slow)			10	N2O5 + HV = NO3 + NO + O3P
16		(Slow)			10	N2O5 + HV = NO3 + NO2
17	6.56e-16	4.50e-14	2.50		11	NO2 + NO3 = NO + NO2 + O2
18		Phot Set= NO3NO			1,12,13	NO3 + HV = NO + O2
19		Phot Set= NO3NO2			1,12,13	NO3 + HV = NO2 + O3P
20		Phot Set= O3O3P			1,14,15	O3 + HV = O3P + O2
21		Phot Set= O3O1D			1,14,15	O3 + HV = O*1D2 + O2
22	2.20e-10	2.20e-10			4	O*1D2 + H2O = #2 HO.
23	2.87e-11	2.09e-11	-0.19		16	O*1D2 + M = O3P + M
24	7.41e-12	Falloff, F=0.60			17	HO. + NO = HONO
	0:	7.00e-31	0.00	-2.6		
	inf:	3.60e-11	0.00	-0.1		
25		Phot Set= HONO-NO			1,18,19	HONO + HV = HO. + NO
26		Phot Set= HONO-NO2			1,18,19	HONO + HV = HO2. + NO2
27	6.46e-12	2.70e-12	-0.52		6	HO. + HONO = H2O + NO2
28	8.98e-12	Falloff, F=0.60			20	HO. + NO2 = HNO3
	0:	2.43e-30	0.00	-3.1		
	inf:	1.67e-11	0.00	-2.1		
29	2.00e-11	2.00e-11			6,21	HO. + NO3 = HO2. + NO2
30	1.47e-13	k = k0+k3M/(1+k3M/k2)			22,23	HO. + HNO3 = H2O + NO3
	k0:	7.20e-15	-1.56	0.0		
	k2:	4.10e-16	-2.86	0.0		
	k3:	1.90e-33	-1.44	0.0		
31		Phot Set= HNO3			1,24	HNO3 + HV = HO. + NO2
32	2.09e-13	k = k1 + k2 [M]			25	HO. + CO = HO2. + CO2
	k1:	1.30e-13	0.00	0.0		
	k2:	3.19e-33	0.00	0.0		
33	6.63e-14	1.90e-12	1.99		6	HO. + O3 = HO2. + O2

Table A-2 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
34	8.41e-12	3.40e-12	-0.54		6	HO2. + NO = HO. + NO2
35	1.38e-12	Falloff, F=0.60			6	HO2. + NO2 = HNO4
	0:	1.80e-31	0.00	-3.2		
	inf:	4.70e-12	0.00	0.0		
36	7.55e-2	Falloff, F=0.50			6	HNO4 = HO2. + NO2
	0:	4.10e-5	21.16	0.0		
	inf:	5.70e+15	22.20	0.0		
37		Phot Set= HO2NO2			1,26	HNO4 + HV = #.61 {HO2. + NO2} + #.39 {HO. + NO3}
38	5.02e-12	1.50e-12	-0.72		6	HNO4 + HO. = H2O + NO2 + O2
39	1.87e-15	1.40e-14	1.19		6	HO2. + O3 = HO. + #2 O2
40A	2.87e-12	k = k1 + k2 [M]			27	HO2. + HO2. = HO2H + O2
	k1:	2.20e-13	-1.19	0.0		
	k2:	1.85e-33	-1.95	0.0		
40B	6.46e-30	k = k1 + k2 [M]			27	HO2. + HO2. + H2O = HO2H + O2 + H2O
	k1:	3.08e-34	-5.56	0.0		
	k2:	2.59e-54	-6.32	0.0		
41	4.00e-12	4.00e-12			28	NO3 + HO2. = #.8 {HO. + NO2 + O2} + #.2 {HNO3 + O2}
42	2.28e-16	8.50e-13	4.87		29	NO3 + NO3 = #2 NO2 + O2
43		Phot Set= H2O2			1,30	HO2H + HV = #2 HO.
44	1.70e-12	2.90e-12	0.32		6	HO2H + HO. = HO2. + H2O
45	1.11e-10	4.80e-11	-0.50		6	HO. + HO2. = H2O + O2
S2OH	9.77e-13	Falloff, F=0.45			6,31	HO. + SO2 = HO2. + SULF
	0:	4.00e-31	0.00	-3.3		
	inf:	2.00e-12	0.00	0.0		
H2OH	6.70e-15	7.70e-12	4.17		4	HO. + H2 = HO2. + H2O
Methyl peroxy and methoxy reactions						
MER1	7.29e-12	2.80e-12	-0.57		32,33	C-O2. + NO = NO2 + HCHO + HO2.
MER4	5.21e-12	3.80e-13	-1.55		32	C-O2. + HO2. = COOH + O2
MEN3	1.30e-12	1.30e-12			32	C-O2. + NO3 = HCHO + HO2. + NO2
MER5	2.65e-13	2.45e-14	-1.41		34	C-O2. + C-O2. = MEOH + HCHO + O2
MER6	1.07e-13	5.90e-13	1.01		34	C-O2. + C-O2. = #2 {HCHO + HO2.}
Peroxy Racical Operators						
RRNO	9.04e-12	2.70e-12	-0.72		35,36,33	RO2-R. + NO = NO2 + HO2.
RRH2	1.49e-11	1.90e-13	-2.58		36,37	RO2-R. + HO2. = ROOH + O2 + #-3 XC
RRN3	2.30e-12	2.30e-12			38,39	RO2-R. + NO3 = NO2 + O2 + HO2.
RRME	2.00e-13	2.00e-13			40,41	RO2-R. + C-O2. = HO2. + #.75 HCHO + #.25 MEOH
RRR2	3.50e-14	3.50e-14			42,41	RO2-R. + RO2-R. = HO2.
R2NO	Same k as rxn RRNO				43,44	R2O2. + NO = NO2
R2H2	Same k as rxn RRH2				43,44	R2O2. + HO2. = HO2.
R2N3	Same k as rxn RRN3				43,44	R2O2. + NO3 = NO2
R2ME	Same k as rxn RRME				43,44	R2O2. + C-O2. = C-O2.
R2RR	Same k as rxn RRR2				43,44,41	R2O2. + RO2-R. = RO2-R.
R2R3	Same k as rxn RRR2				43,44	R2O2. + R2O2. =
RNNO	Same k as rxn RRNO				43,45	RO2-N. + NO = RNO3
RNH2	Same k as rxn RRH2				43,45,46	RO2-N. + HO2. = ROOH + #3 XC

Table A-2 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
RNME	Same k as rxn RRME				43,45,47	RO2-N. + C-O2. = HO2. + #.25 MEOH + #.5 {MEK + PROD2} + #.75 HCHO + XC
RNN3	Same k as rxn RRN3				43,45,48	RO2-N. + NO3 = NO2 + O2 + HO2. + MEK + #2 XC
RNRR	Same k as rxn RRR2				43,45,47	RO2-N. + RO2-R. = HO2. + #.5 {MEK + PROD2} + O2 + XC
RNR2	Same k as rxn RRR2				43,44	RO2-N. + R2O2. = RO2-N.
RNRN	Same k as rxn RRR2				43,45,47	RO2-N. + RO2-N. = MEK + HO2. + PROD2 + O2 + #2 XC
Reactions of Acyl Peroxy Radicals, PAN, and PAN analogues						
APN2	1.05e-11	Falloff, F=0.30			49	CCO-O2. + NO2 = PAN
	0:	2.70e-28	0.00	-7.1		
	inf:	1.20e-11	0.00	-0.9		
DPAN	5.21e-4	Falloff, F=0.30			50	PAN = CCO-O2. + NO2
	0:	4.90e-3	24.05	0.0		
	inf:	4.00e+16	27.03	0.0		
APNO	2.13e-11	7.80e-12	-0.60		51	CCO-O2. + NO = C-O2. + CO2 + NO2
APH2	1.41e-11	4.30e-13	-2.07		52	CCO-O2. + HO2. = #.75 {CCO-OOH +O2} + #.25 {CCO-OH + O3}
APN3	4.00e-12	4.00e-12			53	CCO-O2. + NO3 = C-O2. + CO2 + NO2 + O2
APME	9.64e-12	1.80e-12	-0.99		54	CCO-O2. + C-O2. = CCO-OH + HCHO + O2
APRR	7.50e-12	7.50e-12			55,56	CCO-O2. + RO2-R. = CCO-OH
APR2	Same k as rxn APRR				43,44	CCO-O2. + R2O2. = CCO-O2.
APRN	Same k as rxn APRR				43,56,47	CCO-O2. + RO2-N. = CCO-OH + PROD2
APAP	1.55e-11	2.90e-12	-0.99		32	CCO-O2. + CCO-O2. = #2 {C-O2. + CO2} + O2
PPN2	1.21e-11	1.20e-11	0.00	-0.9	57,58	RCO-O2. + NO2 = PAN2
PAN2	4.43e-4	2.00e+15	25.44		59,58	PAN2 = RCO-O2. + NO2
PPNO	2.80e-11	1.25e-11	-0.48		60,58	RCO-O2. + NO = NO2 + CCHO + RO2-R. + CO2
PPH2	Same k as rxn APH2				61,58	RCO-O2. + HO2. = #.75 {RCO-OOH + O2} + #.25 {RCO-OH + O3}
PPN3	Same k as rxn APN3				61,58	RCO-O2. + NO3 = NO2 + CCHO + RO2-R. + CO2 + O2
PPME	Same k as rxn APME				61,58	RCO-O2. + C-O2. = RCO-OH + HCHO + O2
PPRR	Same k as rxn APRR				61,58	RCO-O2. + RO2-R. = RCO-OH + O2
PPR2	Same k as rxn APRR				61,44	RCO-O2. + R2O2. = RCO-O2.
PPRN	Same k as rxn APRR				61,47,58	RCO-O2. + RO2-N. = RCO-OH + PROD2 + O2
PPAP	Same k as rxn APAP				61,58	RCO-O2. + CCO-O2. = #2 CO2 + C-O2. + CCHO + RO2-R. + O2
PPPP	Same k as rxn APAP				61,58	RCO-O2. + RCO-O2. = #2 {CCHO + RO2-R. + CO2}
BPN2	1.37e-11	1.37e-11			62	BZCO-O2. + NO2 = PBZN
BPAN	3.12e-4	7.90e+16	27.82		63	PBZN = BZCO-O2. + NO2
BPNO	Same k as rxn PPNO				64,65	BZCO-O2. + NO = NO2 + CO2 + BZ-O. + R2O2.
BPH2	Same k as rxn APH2				64,65	BZCO-O2. + HO2. = #.75 {RCO-OOH + O2} + #.25 {RCO-OH + O3} + #4 XC
BPN3	Same k as rxn APN3				64,65	BZCO-O2. + NO3 = NO2 + CO2 + BZ-O. + R2O2. + O2
BPME	Same k as rxn APME				64,65	BZCO-O2. + C-O2. = RCO-OH + HCHO + O2 + #4 XC
BPRR	Same k as rxn APRR				64,65	BZCO-O2. + RO2-R. = RCO-OH + O2 + #4 XC
BPR2	Same k as rxn APRR				44,64	BZCO-O2. + R2O2. = BZCO-O2.

Table A-2 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
BPRN	Same k as rxn APRR				47,64,65	BZCO-O2. + RO2-N. = RCO-OH + PROD2 + O2 + #4 XC
BPAP	Same k as rxn APAP				64,65	BZCO-O2. + CCO-O2. = #2 CO2 + C-O2. + BZ-O. + R2O2.
BPPP	Same k as rxn APAP				64,58,65	BZCO-O2. + RCO-O2. = #2 CO2 + CCHO + RO2-R. + BZ-O. + R2O2.
BPBP	Same k as rxn APAP				64,65	BZCO-O2. + BZCO-O2. = #2 {BZ-O. + R2O2. + CO2}
MPN2	Same k as rxn PPN2				64,66	MA-RCO3. + NO2 = MA-PAN
MPPN	3.55e-4	1.60e+16	26.80		67	MA-PAN = MA-RCO3. + NO2
MPNO	Same k as rxn PPNO				64,66	MA-RCO3. + NO = NO2 + CO2 + HCHO + CCO-O2.
MPH2	Same k as rxn APH2				64,66	MA-RCO3. + HO2. = #.75 {RCO-OOH + O2} + #.25 {RCO-OH + O3} + XC
MPN3	Same k as rxn APN3				64,66	MA-RCO3. + NO3 = NO2 + CO2 + HCHO + CCO-O2. + O2
MPME	Same k as rxn APME				64,66	MA-RCO3. + C-O2. = RCO-OH + HCHO + XC + O2
MPRR	Same k as rxn APRR				64,66	MA-RCO3. + RO2-R. = RCO-OH + XC
MPR2	Same k as rxn APRR				44,64	MA-RCO3. + R2O2. = MA-RCO3.
MPRN	Same k as rxn APRR				64,66	MA-RCO3. + RO2-N. = #2 RCO-OH + O2 + #4 XC
MPAP	Same k as rxn APAP				64,66	MA-RCO3. + CCO-O2. = #2 CO2 + C-O2. + HCHO + CCO-O2. + O2
MPPP	Same k as rxn APAP				64,66	MA-RCO3. + RCO-O2. = HCHO + CCO-O2. + CCHO + RO2-R. + #2 CO2
MPBP	Same k as rxn APAP				64,66	MA-RCO3. + BZCO-O2. = HCHO + CCO-O2. + BZ-O. + R2O2. + #2 CO2
MPMP	Same k as rxn APAP				64,66	MA-RCO3. + MA-RCO3. = #2 {HCHO + CCO-O2. + CO2}
Other Organic Radical Species						
TBON	2.40e-11	2.40e-11			68,69	TBU-O. + NO2 = RNO3 + #-2 XC
TBOD	9.87e+2	7.50e+14	16.20		70,69	TBU-O. = ACET + C-O2.
BRN2	3.80e-11	2.30e-11	-0.30		71	BZ-O. + NO2 = NPHE
BRH2	Same k as rxn RRH2				72	BZ-O. + HO2. = PHEN
BRXX	1.00e-3	1.00e-3			73	BZ-O. = PHEN
BNN2	Same k as rxn BRN2				74	BZ(NO2)-O. + NO2 = #2 XN + #6 XC
BNH2	Same k as rxn RRH2				72	BZ(NO2)-O. + HO2. = NPHE
BNXX	Same k as rxn BRXX				73	BZ(NO2)-O. = NPHE
Explicit and Lumped Molecule Organic Products						
FAHV	Phot Set= HCHO_R				75	HCHO + HV = #2 HO2. + CO
FAVS	Phot Set= HCHO_M				75	HCHO + HV = H2 + CO
FAOH	9.20e-12	8.60e-12	-0.04		32	HCHO + HO. = HO2. + CO + H2O
FAH2	7.90e-14	9.70e-15	-1.24		32	HCHO + HO2. = HOCOO.
FAHR	1.51e+2	2.40e+12	13.91		32	HOCOO. = HO2. + HCHO
FAHN	Same k as rxn MER1				76	HOCOO. + NO = HCOOH + NO2 + HO2.
FAN3	5.74e-16	2.00e-12	4.83		77	HCHO + NO3 = HNO3 + HO2. + CO
AAOH	1.58e-11	5.60e-12	-0.62		32	CCHO + HO. = CCO-O2. + H2O
AAHV	Phot Set= CCHO_R				78	CCHO + HV = CO + HO2. + C-O2.
AAN3	2.73e-15	1.40e-12	3.70		79	CCHO + NO3 = HNO3 + CCO-O2.

Table A-2 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
PAOH	2.00e-11	2.00e-11			80,32,81, 82	RCHO + HO. = #.034 RO2-R. + #.001 RO2-N. + #.965 RCO-O2. + #.034 CO + #.034 CCHO + #-0.003 XC
PAHV	Phot Set= C2CHO				80,78	RCHO + HV = CCHO + RO2-R. + CO + HO2.
PAN3	3.67e-15	1.40e-12	3.52		80,83	RCHO + NO3 = HNO3 + RCO-O2.
K3OH	1.92e-13	1.10e-12	1.03		32,84	ACET + HO. = HCHO + CCO-O2. + R2O2.
K3HV	Phot Set= ACETONE				85	ACET + HV = CCO-O2. + C-O2.
K4OH	1.18e-12	1.30e-12	0.05	2.0	32,81,82	MEK + HO. = #.37 RO2-R. + #.042 RO2-N. + #.616 R2O2. + #.492 CCO-O2. + #.096 RCO-O2. + #.115 HCHO + #.482 CCHO + #.37 RCHO + #.287 XC
K4HV	Phot Set= KETONE, qy= 1.5e-1				86	MEK + HV = CCO-O2. + CCHO + RO2-R.
MeOH	9.14e-13	3.10e-12	0.72	2.0	87	MEOH + HO. = HCHO + HO2.
MER9	5.49e-12	2.90e-12	-0.38		88	COOH + HO. = H2O + #.35 {HCHO + HO.} + #.65 C-O2.
MERA	Phot Set= COOH				89	COOH + HV = HCHO + HO2. + HO.
LPR9	1.10e-11	1.10e-11			90,91	ROOH + HO. = H2O + RCHO + #.34 RO2-R. + #.66 HO.
LPRA	Phot Set= COOH				92	ROOH + HV = RCHO + HO2. + HO.
GLHV	Phot Set= GLY_R				93,94	GLY + HV = #2 {CO + HO2.}
GLVM	Phot Set= GLY_ABS, qy= 6.0e-3				93,95	GLY + HV = HCHO + CO
GLOH	1.10e-11	1.10e-11			32,96,97	GLY + HO. = #.63 HO2. + #1.26 CO + #.37 RCO-O2. + #-.37 XC
GLN3	9.63e-16	2.80e-12	4.72		97,98	GLY + NO3 = HNO3 + #.63 HO2. + #1.26 CO + #.37 RCO-O2. + #-.37 XC
MGHV	Phot Set= MGLY_ADJ				99	MGLY + HV = HO2. + CO + CCO-O2.
MGOH	1.50e-11	1.50e-11			32	MGLY + HO. = CO + CCO-O2.
MGN3	2.43e-15	1.40e-12	3.77		98	MGLY + NO3 = HNO3 + CO + CCO-O2.
BAHV	Phot Set= BACL_ADJ				100,101	BACL + HV = #2 CCO-O2.
PHOH	2.63e-11	2.63e-11			102,103	PHEN + HO. = #.24 BZ-O. + #.76 RO2-R. + #.23 GLY + #4.1 XC
PHN3	3.78e-12	3.78e-12			102,104	PHEN + NO3 = HNO3 + BZ-O.
CROH	4.20e-11	4.20e-11			102,105	CRES + HO. = #.24 BZ-O. + #.76 RO2-R. + #.23 MGLY + #4.87 XC
CRN3	1.37e-11	1.37e-11			102,104	CRES + NO3 = HNO3 + BZ-O. + XC
NPN3	Same k as rxn PHN3				106	NPHE + NO3 = HNO3 + BZ(NO2)-O.
BZOH	1.29e-11	1.29e-11			102	BALD + HO. = BZCO-O2.
BZHV	Phot Set= BZCHO, qy= 5.0e-2				107	BALD + HV = #7 XC
BZNT	2.62e-15	1.40e-12	3.72		108	BALD + NO3 = HNO3 + BZCO-O2.
MAOH	3.36e-11	1.86e-11	-0.35		109,82, 110	METHACRO + HO. = #.5 RO2-R. + #.416 CO + #.084 HCHO + #.416 MEK + #.084 MGLY + #.5 MA-RCO3. + #-0.416 XC
MAO3	1.13e-18	1.36e-15	4.20		109,111, 112,113	METHACRO + O3 = #.008 HO2. + #.1 RO2-R. + #.208 HO. + #.1 RCO-O2. + #.45 CO + #.117 CO2 + #.2 HCHO + #.9 MGLY + #.333 HCOOH + #-0.1 XC
MAN3	4.58e-15	1.50e-12	3.43		109,114, 82,115	METHACRO + NO3 = #.5 {HNO3 + RO2-R. + CO +MA-RCO3.} + #1.5 XC + #.5 XN

Table A-2 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
MAOP	6.34e-12	6.34e-12			116,5	METHACRO + O3P = RCHO + XC
MAHV	Phot Set= ACROLEIN, qy= 4.1e-3				109,117	METHACRO + HV = #.34 HO2. + #.33 RO2-R. + #.33 HO. + #.67 CCO-O2. + #.67 CO + #.67 HCHO + #.33 MA-RCO3. + #-0 XC
MVOH	1.89e-11	4.14e-12	-0.90		109,82	MVK + HO. = #.3 RO2-R. + #.025 RO2-N. + #.675 R2O2. + #.675 CCO-O2. + #.3 HCHO + #.675 RCHO + #.3 MGLY + #-0.725 XC
MVO3	4.58e-18	7.51e-16	3.02		109,111, 112,82 113	MVK + O3 = #.064 HO2. + #.05 RO2-R. + #.164 HO. + #.05 RCO-O2. + #.475 CO + #.124 CO2 + #.1 HCHO + #.95 MGLY + #.351 HCOOH + #-0.05 XC
MVN3		(Slow)			109	MVK + NO3 = #4 XC + XN
MVOP	4.32e-12	4.32e-12			116,5	MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC
MVHV	Phot Set= ACROLEIN, qy= 2.1e-3				109,117, 118	MVK + HV = #.3 C-O2. + #.7 CO + #.7 PROD2 + #.3 MA-RCO3. + #-2.4 XC
IPOH	6.19e-11	6.19e-11			119,109, 82	ISO-PROD + HO. = #.67 RO2-R. + #.041 RO2-N. + #.289 MA-RCO3. + #.336 CO + #.055 HCHO + #.129 CCHO + #.013 RCHO + #.15 MEK + #.332 PROD2 + #.15 GLY + #.174 MGLY + #-0.504 XC
IPO3	4.18e-18	4.18e-18			119,109, 82,120, 112,121, 113	ISO-PROD + O3 = #.4 HO2. + #.048 RO2-R. + #.048 RCO-O2. + #.285 HO. + #.498 CO + #.14 CO2 + #.125 HCHO + #.047 CCHO + #.21 MEK + #.023 GLY + #.742 MGLY + #.1 HCOOH + #.372 RCO-OH + #-.33 XC
IPN3	1.00e-13	1.00e-13			119,109, 82	ISO-PROD + NO3 = #.799 RO2-R. + #.051 RO2-N. + #.15 MA-RCO3. + #.572 CO + #.15 HNO3 + #.227 HCHO + #.218 RCHO + #.008 MGLY + #.572 RNO3 + #.28 XN + #-.815 XC
IPHV	Phot Set= ACROLEIN, qy= 4.1e-3				119,109, 82,122	ISO-PROD + HV = #1.233 HO2. + #.467 CCO-O2. + #.3 RCO-O2. + #1.233 CO + #.3 HCHO + #.467 CCHO + #.233 MEK + #-.233 XC
<u>Lumped Parameter Organic Products</u>						
K6OH	1.50e-11	1.50e-11			123	PROD2 + HO. = #.379 HO2. + #.473 RO2-R. + #.07 RO2-N. + #.029 CCO-O2. + #.049 RCO-O2. + #.213 HCHO + #.084 CCHO + #.558 RCHO + #.115 MEK + #.329 PROD2 + #.886 XC
K6HV	Phot Set= KETONE, qy= 2.0e-2				123,124	PROD2 + HV = #.96 RO2-R. + #.04 RO2-N. + #.515 R2O2. + #.667 CCO-O2. + #.333 RCO-O2. + #.506 HCHO + #.246 CCHO + #.71 RCHO + #.299 XC
RNOH	7.80e-12	7.80e-12			125	RNO3 + HO. = #.338 NO2 + #.113 HO2. + #.376 RO2-R. + #.173 RO2-N. + #.596 R2O2. + #.01 HCHO + #.439 CCHO + #.213 RCHO + #.006 ACET + #.177 MEK + #.048 PROD2 + #.31 RNO3 + #.351 XN + #.56 XC
RNHV	Phot Set= IC3ONO2				125,126	RNO3 + HV = NO2 + #.341 HO2. + #.564 RO2-R. + #.095 RO2-N. + #.152 R2O2. + #.134 HCHO + #.431 CCHO + #.147 RCHO + #.02 ACET + #.243 MEK + #.435 PROD2 + #.35 XC

Table A-2 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [b]	Reaction and Products [c]
Uncharacterized Reactive Aromatic Ring Fragmentation Products						
D1OH	5.00e-11	5.00e-11			127,128	DCB1 + HO. = RCHO + RO2-R. + CO
D1HV		(Slow)			127,129	DCB1 + HV = HO2. + #2 CO + RO2-R. + GLY + R2O2.
D1O3	2.00e-18	2.00e-18			127,130, 120	DCB1 + O3 = #1.5 HO2. + #.5 HO. + #1.5 CO + #.5 CO2 + GLY
D2OH	5.00e-11	5.00e-11			131,132	DCB2 + HO. = R2O2. + RCHO + CCO-O2.
D2HV	Phot Set= MGLY_ABS, qy= 3.7e-1				131,133	DCB2 + HV = RO2-R. + #.5 {CCO-O2. + HO2.} + CO + R2O2. + #.5 {GLY + MGLY + XC}
D3OH	5.00e-11	5.00e-11			131,132	DCB3 + HO. = R2O2. + RCHO + CCO-O2.
D3HV	Phot Set= ACROLEIN, qy= 7.3e+0				131,133	DCB3 + HV = RO2-R. + #.5 {CCO-O2. + HO2.} + CO + R2O2. + #.5 {GLY + MGLY + XC}

[a] Except as indicated, the rate constants are given by $k(T) = A \cdot (T/300)^{B} \cdot e^{-Ea/RT}$, where the units of k and A are cm^3 $molec^{-1}$ s^{-1}, Ea are kcal mol^{-1}, T is ^oK, and R=0.0019872 kcal mol^{-1} deg^{-1}. The following special rate constant expressions are used:

Phot Set = *name*: The absorption cross sections and quantum yields for the photolysis reaction are given in Table A-5, where "*name*" indicates the photolysis set used. If a "qy=*number*" notation is given, the number given is the overall quantum yield, which is assumed to be wavelength independent.

Falloff: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = \{k0(T)\cdot[M]/[1 + k0(T)\cdot[M]/kinf(T)]\}\cdot F^{Z}$, where $Z = \{1 + [\log_{10}\{k0(T)\cdot[M])/kinf(T)\}]^2\}^{-1}$, [M] is the total pressure in molecules cm^{-3}, F is as indicated on the table, and the temperature dependences of k0 and kinf are as indicated on the table.

(Slow): The reaction is assumed to be negligible and is not included in the mechanism. It is shown on the listing for documentation purposes only.

k = k0+k3M(1+k3M/k2): The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k0(T) + k3(T)\cdot[M] \cdot(1 + k3(T)\cdot[M]/k2(T))$, where [M] is the total bath gas (air) concentration in molecules cm^{-3}, and the temperature dependences for k0, k2 and k3 are as indicated on the table.

k = k1 + k2 [M]: The rate constant as a function of temperature and pressure is calculated using $k(T,M) = k1(T) + k2(T)\cdot[M]$, where [M] is the total bath gas (air) concentration in molecules cm^{-3}, and the temperature dependences for k1, and k2 are as indicated on the table.

Same k as Rxn *label*: The rate constant is the same as the reaction with the indicated label.

[c] Footnotes given in Table A-3.

[b] Format of reaction listing: "=" separates reactants from products; "*#number*" indicates stoichiometric coefficient, "*#coefficient* { *product list* }" means that the stoichiometric coefficient is applied to all the products listed.

Table A-3. Listing and documentation of reactions added to the base mechanism to constitute the fixed parameter lumped mechanism.

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [a]	Reaction and Products [a]
Explicitly Represented Primary Organics						
c1OH	6.37e-15	2.15e-12	3.45		32	CH4 + HO. = H2O + C-O2.
etOH	8.52e-12	1.96e-12	-0.87		134	ETHENE + HO. = RO2-R. + #1.61 HCHO + #.195 CCHO
etO3	1.59e-18	9.14e-15	5.13		134	ETHENE + O3 = #.12 HO. + #.12 HO2. + #.5 CO + #.13 CO2 + HCHO + #.37 HCOOH
etN3	2.05e-16	4.39e-13	4.53	2.0	134	ETHENE + NO3 = RO2-R. + RCHO + #-1 XC + XN
etOA	7.29e-13	1.04e-11	1.57		134	ETHENE + O3P = #.5 HO2. + #.2 RO2-R. + #.3 C-O2. + #.491 CO + #.191 HCHO + #.25 CCHO + #.009 GLY + #.5 XC
isOH	9.82e-11	2.50e-11	-0.81		134,135	ISOPRENE + HO. = #.907 RO2-R. + #.093 RO2-N. + #.079 R2O2. + #.624 HCHO + #.23 METHACRO + #.32 MVK + #.357 ISO-PROD + #-0.167 XC
isO3	1.28e-17	7.86e-15	3.80		134,135	ISOPRENE + O3 = #.266 HO. + #.066 RO2-R. + #.008 RO2-N. + #.126 R2O2. + #.192 MA-RCO3. + #.275 CO + #.122 CO2 + #.592 HCHO + #.1 PROD2 + #.39 METHACRO + #.16 MVK + #.204 HCOOH + #.15 RCO-OH + #-0.259 XC
isN3	6.74e-13	3.03e-12	0.89		134,135	ISOPRENE + NO3 = #.187 NO2 + #.749 RO2-R. + #.064 RO2-N. + #.187 R2O2. + #.936 ISO-PROD + #-0.064 XC + #.813 XN
isOP	3.60e-11	3.60e-11			134,135	ISOPRENE + O3P = #.01 RO2-N. + #.24 R2O2. + #.25 C-O2. + #.24 MA-RCO3. + #.24 HCHO + #.75 PROD2 + #-1.01 XC
Lumped Terpenes (Based on estimated North America annual emissions rate of top 5 terpenes.)						
t1OH	8.27e-11	1.83e-11	-0.89		134,136	TERP + HO. = #.75 RO2-R. + #.25 RO2-N. + #.5 R2O2. + #.276 HCHO + #.474 RCHO + #.276 PROD2 + #5.146 XC
t1O3	6.88e-17	1.08e-15	1.63		134,136	TERP + O3 = #.567 HO. + #.033 HO2. + #.031 RO2-R. + #.18 RO2-N. + #.729 R2O2. + #.123 CCO-O2. + #.201 RCO-O2. + #.157 CO + #.037 CO2 + #.235 HCHO + #.205 RCHO + #.13 ACET + #.276 PROD2 + #.001 GLY + #.031 BACL + #.103 HCOOH + #.189 RCO-OH + #4.183 XC
t1N3	6.57e-12	3.66e-12	-0.35		134,136	TERP + NO3 = #.474 NO2 + #.276 RO2-R. + #.25 RO2-N. + #.75 R2O2. + #.474 RCHO + #.276 RNO3 + #5.421 XC + #.25 XN
t1OP	3.27e-11	3.27e-11			134,136	TERP + O3P = #.147 RCHO + #.853 PROD2 + #4.441 XC
Lumped Primary Organics (Based on base ROG mixture used in reactivity scenarios)						
a1OH	2.54e-13	1.37e-12	0.99	2.0	134,137	ALK1 + HO. = RO2-R. + CCHO
a2OH	1.04e-12	9.87e-12	1.33		134,138	ALK2 + HO. = #.246 HO. + #.121 HO2. + #.612 RO2-R. + #.021 RO2-N. + #.16 CO + #.039 HCHO + #.155 RCHO + #.417 ACET + #.248 GLY + #.121 HCOOH + #0.338 XC
a3OH	2.38e-12	1.02e-11	0.86		134,139	ALK3 + HO. = #.695 RO2-R. + #.07 RO2-N. + #.559 R2O2. + #.236 TBU-O. + #.026 HCHO + #.445 CCHO + #.122 RCHO + #.024 ACET + #.332 MEK + #-0.05 XC

Table A-3 (continued)

Label	Rate Parameters [a] k(298)	A	Ea	B	Refs & Notes [a]	Reaction and Products [a]
a4OH	4.39e-12	5.95e-12	0.18		134,139	ALK4 + HO. = #.835 RO2-R. + #.143 RO2-N. + #.936 R2O2. + #.011 C-O2. + #.011 CCO-O2. + #.002 CO + #.024 HCHO + #.455 CCHO + #.244 RCHO + #.452 ACET + #.11 MEK + #.125 PROD2 + #-0.105 XC
a5OH	9.34e-12	1.11e-11	0.10		134,139	ALK5 + HO. = #.653 RO2-R. + #.347 RO2-N. + #.948 R2O2. + #.026 HCHO + #.099 CCHO + #.204 RCHO + #.072 ACET + #.089 MEK + #.417 PROD2 + #2.008 XC
b1OH	5.95e-12	1.81e-12	-0.71		134,140	ARO1 + HO. = #.224 HO2. + #.765 RO2-R. + #.011 RO2-N. + #.055 PROD2 + #.118 GLY + #.119 MGLY + #.017 PHEN + #.207 CRES + #.059 BALD + #.491 DCB1 + #.108 DCB2 + #.051 DCB3 + #1.288 XC
b2OH	2.64e-11	2.64e-11	0.00		134,139	ARO2 + HO. = #.187 HO2. + #.804 RO2-R. + #.009 RO2-N. + #.097 GLY + #.287 MGLY + #.087 BACL + #.187 CRES + #.05 BALD + #.561 DCB1 + #.099 DCB2 + #.093 DCB3 + #1.68 XC
o1OH	3.23e-11	7.10e-12	-0.90		134,139	OLE1 + HO. = #.91 RO2-R. + #.09 RO2-N. + #.205 R2O2. + #.732 HCHO + #.294 CCHO + #.497 RCHO + #.005 ACET + #.119 PROD2 + #.92 XC
o1O3	1.06e-17	2.62e-15	3.26		134,139	OLE1 + O3 = #.155 HO. + #.056 HO2. + #.022 RO2-R. + #.001 RO2-N. + #.076 C-O2. + #.345 CO + #.086 CO2 + #.5 HCHO + #.154 CCHO + #.363 RCHO + #.001 ACET + #.215 PROD2 + #.185 HCOOH + #.05 CCO-OH + #.119 RCO-OH + #.654 XC
o1N3	1.26e-14	4.45e-14	0.75		134,139	OLE1 + NO3 = #.824 RO2-R. + #.176 RO2-N. + #.488 R2O2. + #.009 CCHO + #.037 RCHO + #.024 ACET + #.511 RNO3 + #.677 XC + #.489 XN
o1OP	4.90e-12	1.07e-11	0.47		134,139	OLE1 + O3P = #.45 RCHO + #.437 MEK + #.113 PROD2 + #1.224 XC
o2OH	6.33e-11	1.74e-11	-0.76		134,139	OLE2 + HO. = #.918 RO2-R. + #.082 RO2-N. + #.001 R2O2. + #.244 HCHO + #.732 CCHO + #.511 RCHO + #.127 ACET + #.072 MEK + #.061 BALD + #.025 METHACRO + #.025 ISO-PROD + #-.054 XC
o2O3	1.07e-16	5.02e-16	0.92		134,139	OLE2 + O3 = #.378 HO. + #.003 HO2. + #.033 RO2-R. + #.002 RO2-N. + #.137 R2O2. + #.197 C-O2. + #.137 CCO-O2. + #.006 RCO-O2. + #.265 CO + #.07 CO2 + #.269 HCHO + #.456 CCHO + #.305 RCHO + #.045 ACET + #.026 MEK + #.006 PROD2 + #.042 BALD + #.026 METHACRO + #.073 HCOOH + #.129 CCO-OH + #.303 RCO-OH + #.155 XC
o2N3	7.27e-13	7.27e-13	0.00		134,139	OLE2 + NO3 = #.391 NO2 + #.442 RO2-R. + #.136 RO2-N. + #.711 R2O2. + #.03 C-O2. + #.079 HCHO + #.507 CCHO + #.151 RCHO + #.102 ACET + #.001 MEK + #.015 BALD + #.048 MVK + #.321 RNO3 + #.075 XC + #.288 XN
o2OP	2.09e-11	2.09e-11			134,139	OLE2 + O3P = #.013 HO2. + #.012 RO2-R. + #.001 RO2-N. + #.012 CO + #.069 RCHO + #.659 MEK + #.259 PROD2 + #.012 METHACRO + #.537 XC

[a] See footnotes to Table A-2. Documentation text is in Table A-4.

Table A-4. Documentation notes for the base and lumped mechanisms.

No.	Note
1	See Table A-5 for listing of absorption cross sections and quantum yields. Set used is given in the "Type" column.
2	Absorption cross sections and quantum yields from IUPAC recommendation (Atkinson et al, 1997), except that quantum yields for wl > 410 nm are from NASA (1997), which are consistent with IUPAC (Atkinson et al, 1997) values except they are more precise. Note that more recent IUPAC recommendations (Atkinson et al, 1997b) gives slightly different absorption cross sections based on data from a more recent study, but the differences are not significant.
3	Rate constant expression derived from IUPAC (Atkinson et al, 1997b) recommendations for M = 20.9% O2 and 79.1% N2.
4	Rate constant is IUPAC, Supplement VI (Atkinson et al, 1997b) and NASA (1997) recommendation.
5	This reaction is probably not important in the troposphere, but is included to increase range of applicability.
6	Rate constant expression is IUPAC (Atkinson et al, 1997b) recommendation.
7	Recommended rate constant given for N2 is assumed to be applicable to air.
8	The falloff parameters recommended by NASA (1997) give a 300K, 1 atm rate constant which is approximately 13% lower than the IUPAC-recommended values that were used.
9	The data of Mentel et al (1996) indicate that the reaction occurs through pathways that are first order and second order in H2O, where the latter is presumed to be surface-dependent. We assume that the process which is first order in H2O represents a gas-phase reaction, and use the rate expression of Mentel et al (1996) for this process. Note that the IUPAC (Atkinson et al, 1997b) recommendation that the gas-phase rate constant is less than 2×10^{-21} cm-3 molec-1 s-1.
10	Photolysis of N2O5 is assumed to be negligible compared to decomposition under atmospheric conditions.
11	The NASA (1997) evaluation states that the existence of this channel has not been firmly established, but results of a number of studies indicate it may occur. Rate constant expression used is that NASA (1997) states gives best fits to the data. Uncertainty is at least a factor of 2. This reaction was not discussed in the recent IUPAC evaluations (Atkinson et al, 1997).
12	Absorption cross sections from IUPAC (Atkinson et al, 1997). Values recommended by more recent IUPAC evaluation (Atkinson et al, 1997b) appear to be the same for 298K, though different at lower temperature. Temperature dependence ignored.
13	IUPAC (1997b) and NASA (1997) give no useable recommendations for quantum yields except to recommend that qy(NO2+O)=1 for wl <= 583. Quantum yields of Magnotta and Johnsom (1980), scaled down by a factor of 1.5 to give unit maximum quantum yields, as incorporated in mechanism of Carter (1990) were retained in this mechanism. The calculated rate constant for solar overhead sun is consistent with the recommendations of Magnotta and Johnson (1980), and reasonably consistent with the IUPAC (1997) recommendation.
14	Absorption cross sections for the low wavelength region are from the NASA (1997) evaluation, given for T=273K The values given by IUPAC (Atkinson et al, 1997b) appear to be the same, but the notation in the tabulation is unclear. Absorption cross sections for the high wavelength region are from IUPAC (Atkinson et al, 1997b). Temperature dependences for the low wavelength cross sections are ignored.

Table A-4 (continued)

No.	Note
15	Quantum yields for O^1D are those tabulated by IUPAC (Atkinson et al, 1997b), which are significantly higher than previous recommendations at $\lambda > 310$ nm. No recommendation is given for quantum yields for O1D for wavelengths above 335 nm; they are assume to decline linearly to 0 at 340 nm. Quantum yields for O^3P are based on assuming total quantum yield of unity, though this was not adequately discussed in the evaluations.
16	Calculated using IUPAC (Atkinson et al, 1997b) recommended rate constants for reaction with O2 and N2, assuming 20.9% O2 and 79.1% N2. Temperature dependence optimized to fit rate constants calculated for T= 270, 300, and 330K.
17	Falloff expression recommended by NASA (1997) used because it gives rate constant for 1 atm N2 which is consistent with measurement near those conditions. IUPAC (Atkinson et al, 1997) recommendations are not used because k (1 atm N2) are not consistent with these data, being based on high pressure data in He. This is consistent with current recommendation of Atkinson (private communication, 1997).
18	Absorption cross sections from the NASA (1997) evaluation.
19	Quantum yields are those recommended by IUPAC (Atkinson et al, 1997b).
20	NASA (1997) and IUPAC (Atkinson et al, 1997) give significantly different recommendations for rate parameters for this important reaction. The falloff expression used here is based on a NASA (1997) and IUPAC (Atkinson et al, 1997) give significantly different recommendations for rate parameters for this important reaction. The falloff expression used here is based on a re-evaluation of the data by Golden (Personal communication, 1998), and is expected to be the recommendation in the next NASA evaluation. This is essentially the same as the NASA (1997) recommendation except for the temperature dependence, which Golden says was due to improper uncertainty weighting. The data with "weak colliders (i.e., bath gases other than SF6 or CF4) appear to be well fit by this parameterization, including the data of Donahue et al (1997). The data of Forster et al (1995), which are the basis for the high 1997 IUPAC recommendation, are not used because they may be due to a HOONO-forming channel becoming important at high pressures.
21	No recommendation is given concerning the temperature dependence of this rate constant, which is assumed to be small.
22	The rate parameters were derived to fit the rate constants calculated using the NASA (1997) recommended expression for T 270 - 330 K range and 1 atm. total pressure.
23	This rate constant is strictly valid for 1 atm air only, but the error introduced by neglecting the pressure dependence of this reaction is expected to be small.
24	Absorption cross-sections from IUPAC (Atkinson et al, 1997b). Recommend quantum yield for the OH + NO2 pathway is "close to unity" for wl > 260 nm, though other pathways become important at lower wavelengths.
25	The rate constants for the OH + CO reactions are based on expression given by IUPAC (Atkinson et al, 1997). NASA (1997) gives a similar expression, but without temperature dependence.
26	Absorption cross sections and quantum yields from IUPAC (Atkinson et al, 1997b). Quantum yields are uncertain and based on data for a single wavelength only.
27	Reactions and rate constants used for the HO2 + HO2 and HO2 + HO2 + H2O system based on the data of Kircher and Sander (1984) as discussed in the IUPAC (Atkinson et al, 1997b) evaluation.
28	Rate constant recommended by IUPAC (Atkinson et al, 1997b). Measurement of the branching ratios vary, so the mechanism is uncertain. The branching ratio assumed is approximately in the middle of the range given by IUPAC (Atkinson et al, 1997b) and NASA (1997) evaluations, which is 0.6 - 1.0 for the OH-forming channel.

Table A-4 (continued)

No.	Note
29	Rate expression from NASA (1994) evaluation. More recent evaluations neglect this reaction, though it may be non-negligible under some nighttime conditions (Stockwell et al, 1997).
30	Absorption cross sections recommended by IUPAC (Atkinson et al, 1997) used. Quantum yield assumed to be unity.
31	The initially formed $HOSO_2$ is believed to react primarily with O_2, forming HO2 and SO_3 (Stockwell and Calvert, 1983). The SO_3 is assumed to be converted into sulfates, which are represented by the SULF model species.
32	Rate constant expression recommended by IUPAC, Supplement VII (Atkinson et al, 1999).
33	The reaction of NO2 is ignored because it is rapidly reversed by the decomposition of the peroxynitrate, resulting in no net reaction. Calculations not neglecting peroxynitrate formation give essentially the same results. However, this may not be valid in low temperature simulations.
34	Total rate constant and rate constant for methoxy radical formation from IUPAC (Atkinson et al, 1997, 1999) recommendation. Temperature dependence for rate constant for methanol + HCHO formation derived to be consistent with these.
35	The RO2-R. operator represents the effects of peroxy radicals which react with NO to form NO2 and HO2, and also the effects of peroxy radical reactions on other species. Except as indicated, the organic products from this peroxy radical are not represented.
36	Rate constant recommended by Atkinson (1997a) for general peroxy radicals.
37	The organic products from the HO2 reaction are represented by the lumped higher hydroperoxide species. Negative "lost carbons" are added because this is a zero-carbon operator.
38	Rate constant based on that recommenced by IUPAC (Atkinson et al, 1999) for ethyl peroxy + NO3. Formation of alkoxy + NO2 + O2 stated to occur >85% of the time.
39	The reaction is assumed to form the corresponding alkoxy radical. The HO2 represents the radicals regenerated by the alkoxy radical.
40	Based on rate constant for methyl peroxy + ethyl peroxy rate given by Atkinson (1997a). This is near the middle of the range of rate constants given for other methyl peroxy + higher alkyl peroxy radical reactions given by Atkinson (1997a) or Atkinson et al (1997a).
41	Approximately half of the peroxy + peroxy reaction is assumed to form two O2 + alkoxy radicals, where the latter react to form HO_2 and organic products, where the formaldehyde from the methoxy is represented in this reaction. The HO2 represents the radicals regenerated in the fraction of this peroxy radical which reacts in this way. The other half of the time the reaction is assumed to proceed via H-atom transfer, with half of that involving transfer from the methyl peroxy, forming formaldehyde, and the other half involving transfer to the methyl peroxy, forming methanol. Note that the organic products from RO2-R· are not represented in this reaction because this is a “massless” operator.
42	The rate constants for peroxy + peroxy radical reactions can vary by orders of magnitude depending on the type of radical (e.g., Atkinson, 1997), so the value used here must be approximate. The value used is the geometric mean of the values recommended by Atkinson (1997a) for primary + primary and secondary + secondary peroxy radicals.
43	Assumed to have same rate constant as used for general higher peroxy radical (see notes for RO2-R.).
44	The R2O2. operator represents the effects of peroxy radical reactions causing extra NO to NO2 conversions. Its reactions with species other than NO are represented as having no effect other than to consume this operator.

Table A-4 (continued)

No.	Note
45	The RO2-N. operator represents the effects of peroxy radicals which react with NO to form higher organic nitrates (represented by RNO3), and also the effects of peroxy radical reactions on other species. It has five carbons.
46	The organic products from the HO2 reaction are represented by the lumped higher hydroperoxide species. "Lost carbons" are added because this is a five-carbon operator.
47	Approximately half of the peroxy + peroxy reaction for radicals represented by RO2-N. is assumed to form two O2 + alkoxy radicals. The MEK + HO2. represents the products and radicals formed from the alkoxy radical from this species. The other half is assumed to involve disproportionation, forming O2 + and an alcohol and carbonyl compound. These are represented by PROD2.
48	This reaction is assumed to form the corresponding alkoxy radical, which is assumed to react products represented by MEK + HO2.
49	Falloff expression recommended by IUPAC (Atkinson et al, 1997, 1999), based on data of Bridier et al (1991).
50	Falloff expression recommended by IUPAC (Atkinson et al, 1992), based on data of Bridier et al (1991). Note: NASA (1997) also recommends using Bridier et al (1991) data, but gives a revised expression which gives a different k at 298K. Based on new data on PAN decomposition which give a factor of ~2 lower rate 298K rate constants, The more recent IUPAC evaluations (Atkinson et al., 1997, 1999) recommend the a high pressure rate constant expression of 5.4×10^{16} exp(-13830/T), derived by averaging the data. We are staying with the earlier IUPAC Recommendations based on the data of Bridier et al (1991) because it gives good agreement with the data of Tuazon et al (1991a) and is consistent with the NASA (1997) recommended equilibrium constant.
51	Rate constant expression recommended by IUPAC (Atkinson et al, 1999). This is almost the same as the earlier IUPAC(Atkinson et al, 1997) recommended value of 2.0×10^{-11} and close to the NASA (1997) value of 1.8×10^{-11}.
52	Branching ratio and rate constant expression recommended by IUPAC (Atkinson et al, 1997, 1999).
53	Rate constant from Canosa-Mass et al (1996)
54	Rate constant expression recommended by IUPAC (Atkinson et al, 1999) evaluation. As discussed there, the data are inconclusive as to the importance of the competing reaction forming CH3O + CH3CO2 + O2, but the study which indicate that it occurs, which was used in the previous IUPAC (Atkinson et al, 1997) evaluation, indicates that it occurs less than ~15% under atmospheric conditions. Therefore, the reaction is assumed to involve disproportionation 100% of the time.
55	Rate constant is the average of the the IUPAC (Atkinson et al, 1999) recommendations of 1×10^{-11} for the acetyl peroxy + ethyl peroxy reaction and 5×10^{-12} for the acetyl peroxy + $CH_3C(O)CH_2O_2$ reaction.
56	This reaction is assumed to proceed primarily by disproportionation to form the organic acid and a carbonyl compound, based on data for the acetyl peroxy + methyl peroxy reaction.
57	The rate parameters are assumed to be approximately the same as those for the reaction of $CH_3C(O)OO\cdot$ at the high pressure limit. This assumption is employed in the IUPAC (Atkinson et al, 1999) evaluation when deriving the recommended value of the $CH_3CH_2C(O)OO\cdot + NO_2$ rate constant.
58	The products of the reactions of RCO-O2. are based on R=ethyl. Mechanism assumed to be similar to corresponding reaction of acetyl peroxy radicals.
59	Rate parameters based on the IUPAC (Atkinson et al, 1999) recommendation for PPN.

Table A-4 (continued)

No.	Note
60	Rate constant expression based on the data of Seefeld and Kerr (1997), which gives k(PPN2)/k(PPNO) = 2.33±0.38, and the value of k(PPN2) used in the mechanism. This is as recommended by IUPAC (Atkinson et al, 1999).
61	Assumed to have same rate constant as corresponding reaction of $CH_3C(O)OO$.
62	Rate constant based on $k(NO_2)/k(NO)$ ratio measured by Kirchner et al (1992) and the k(NO) used for general higher acyl peroxy radical species.
63	Rate constant expression based on the data of Kirchner et al (1992).
64	Assumed to have the same rate constant and mechanism as used for the general higher acyl peroxy radical or higher PAN analogue
65	The mechanism is assumed to be analogous to the mechanism of the corresponding reaction of acetyl peroxy radicals. Note that the formation of benzyl peroxy radicals results in the formation of phenoxy after 1 NO to NO2 conversion, so it can be represented by BZ-O. + R2O2. The general lumped higher orgainc acid (RCO-OH) and peroxyacid (RCO-OOH) are used to represent the aromatic acids and peroxyacids expected to be formed in the peroxy + peroxy reactions.
66	MA-RCO3. and MA-PAN are used to represent the acyl peroxy radical and PAN analogue formed from any acrolein compound. Their reactions are are based on those formed from methacrolein. Generally, the reaction mechanisms are assumed to be analogous to those for the corresponding reactions of acetyl peroxy radicals. The alkoxy radical is assumed to decompose to CO2 + CH2=CH(.)CH3, while the latter reacts with O2 to form HCHO + CH3CO., as discussed by Carter and Atkinson (1996). The general lumped higher orgainc acid (RCO-OH) and peroxyacid (RCO-OOH) are used to represent the unsaturated acids and peroxyacids expected to be formed in the peroxy + peroxy reactions.
67	Rate parameters from Roberts and Bertman (1992), as used by Carter and Atkinson (1996).
68	The rate expression recommended by Atkinson (1997) for general alkoxy + NO_2 reactions is $2.3x10^{-11}$ exp(+150/T). This is reduced by a factor of 1.58 to be consistent with environmental chamber data, as discussed in a separate note.
69	The effects of isobutane on ozone formation and radical levels in environmental chamber experiments are not consistent with predictions of models which assume the recommended rate constant ratios for the decomposition of t-butoxy radicals relative to reaction with NO_2. The data are better fit if the ratio is increased by a factor of 2.5. The error is assumed to be equally distributed in each rate constant, so they are both adjusted by the a factor of 1.58, which is the square root of 2.5. This rate constant must be considered to be uncertain by at least this amount.
70	Atkinson (1997b) recommends the high-pressure rate expression of 6.0x10+14 exp(-16.2/RT). Batt and Robinson (1987) calculate that at one atmosphere the rate constant is 79% the high pressure limit, giving an estimated rate expression of 4.74x10-14 exp(-16.2/RT). This is increased by a factor of 1.58 to be consistent with environmental chamber data, as discussed in a separate note. This rate constant must be considered to be uncertain by at least this amount.
71	The rate constant is based on the general recommendation of Atkinson (1994) for alkoxy + NO2 reactions at the high pressure limit. Nitrophenol formation has generally been assumed in this reaction (e.g., see Atkinson, 1990; Carter, 1990), presumably via some rearrangement of an initially-formed unstable adduct. However, based on lower than expected yields of nitrophenols in NO3 + cresol and OH + benzaldehyde systems (Atkinson, 1994), this may be an oversimplification.
72	Assumed to have the same rate constant as the reaction of HO2 with peroxy radicals. This may underestimate the actual rate constant because alkoxy radicals tend to be more reactive than peroxy radicals.

Table A-4 (continued)

No.	Note
73	This is included to avoid problems if these radicals are ever formed under conditions where both HO_2 and NO_2 are very low (which is considered to be unlikely under most ambient conditions), and can be considered to represent its reaction with organics present. The rate constant is arbitrary, and is such that this process becomes significant only if $[NO_2] < \sim 3x10^{-6}$ ppm and $[HO_2] < 1x10^{-5}$ ppm.
74	The rate constant is based on the general recommendation of Atkinson (1994) for alkoxy + NO2 reactions at the high pressure limit. The products of this reaction (presumed to be aromatic dinitro compounds) are expected to have very low vapor pressures and are represented as unreactive nitrogen and carbon.
75	Absorption cross sections and quantum yields recommended by IUPAC (Atkinson et al, 1997) used. Absorption cross sections used are those given for T = 285K.
76	Rate constant assumed to be the same as used for methylperoxy + NO.
77	T=298K Rate constant recommended by IUPAC (Atkinson et al, 1979a). Temperature dependence is as estimated by IUPAC (Atkinson et al, 1979a).
78	Absorption cross sections and quantum yields recommended by IUPAC (Atkinson et al, 1997, 1999) used. Reaction assumed to occur primarily by breaking the C-CHO bond. Pathway forming molecular products is assumed to be negligible under atmospheric conditions, based on calculated rate for analogous reaction of acetaldehyde.
79	Rate constant expression recommended by IUPAC, Supplement V (Atkinson et al, 1997).
80	The mechanism for RCHO is based on reactions estimated for propionaldehyde.
81	OH reactions at various positions in the molecule estimated using the group-additivity methods of Kwok and Atkinson (1995), as updated by Kwok et al (1996).
82	Except as indicated by other footnotes, the overall reaction mechanism was derived using the general estimation methods for atmospheric reactions of alkyl, alkyl peroxy, and alkoxy radicals and the automated mechanism generation system as discussed in this report.
83	The rate constant is based on the estimated rate constant for the reaction of NO_3 with propionaldehyde. This is based on the correlation noted by Atkinson (1991) between HO and NO_3 radical H-atom abstraction rate constants, the assumption that the reaction only occurs at the -CHO group, and the estimated rate constant for OH reaction at that group. Atkinson (1991) noted that 298K H abstraction rate constants per abstractable hydrogen are approximately fit by $\ln k_{NO3} \approx 6.498 + 1.611 \ln k_{OH}$, and the rate constant for OH abstraction from the -CHO group estimated by group additivity methods is $k_{OH} = 1.94 \times 10^{-11}$ cm^3 $molec^{-1}$ s^{-1}. These correspond to $k_{NO3} \approx 3.67 \times 10^{-15}$ cm^3 $molec^{-1}$ s^{-1} at 298K. The temperature dependence is derived by assuming the same A factor as that for the reaction of NO_3 with acetaldehyde.
84	Reaction in the presence of NOx is assumed to involve formation of $CH_3C(O)CH2O.$, after one NO to NO2 conversion. Based on the data of Jenkin et al (1993), this radical is believed to rapidly decompose to HCHO + CH3CO.
85	Absorption cross sections and quantum yields used are those recommended by IUPAC (Atkinson et al, 1997) except as noted. The reported quantum yields at 230 and 330 are expected to be high and an estimated correction was made as discussed by Carter et al (1993b). The corrected quantum yield data for wavelengths less than 290 nm were then fit to a smooth curve to estimate the quantum yields for higher wavelengths, with no weight being given to the highly uncertain 330 nm point. As discussed by Carter et al (1993b), using these corrections results in better fits of model calculations to environmental chamber experiments involving acetone.

Table A-4 (continued)

No.	Note
86	The absorption coefficients used for MEK are from Moortgat (Private communication, 1996). The overall MEK quantum yield of 0.15 was found to give best fits to the MEK-NOx and MEK reactivity data our laboratories (Carter et al, 2000a). This is slightly higher than the overall quantum yield of 0.1 used in the previous version of the mechanism, based on fits to UNC outdoor chamber data (Carter, 1990). Using an overall quantum yield was found to give better fits to the data using both xenon arc and blacklight light sources than assuming wavelength-dependence quantum yields such as for acetone. The reaction is assumed to proceed primarily by breaking the weakest CO-C bond.
87	The mechanism and rate constants are as recommended by IUPAC (Atkinson et al, 1997, 1999). 85% of the reaction is believed to involve formation of $\cdot CH_2OH$, with the remainder involving formation of $CH_3O\cdot$. However, both these radicals react primarily with O_2 forming formaldehyde + HO_2, so the overall process is as shown.
88	Rate constant and branching ratio for initial OH reaction based on IUPAC (Atkinson et al, 1997, 1999) recommendation. The .CH2OOH radical is assumed to rapidly decompose to HCHO + OH, based on its high estimated exothermicity.
89	Absorption cross sections from IUPAC (Atkinson et al, 1997, 1999), which also recommends assuming unit total quantum yield, but gives no recommendation as to the exact mechanism. Breaking the O-O bond assumed to be the major pathway.
90	The mechanism for ROOH is based on reactions estimated for n-propyl hydroperoxide.
91	Reaction at the OOH position is assumed to be as fast as in CH3OOH. Reaction at the 1-position is estimated to be ~7x10-12 (i.e., ~2/3 of the time) based on comparing rates of analogous reactions for methanol, ethanol, and CH3OOH (Atkinson et al., 1997, 1999). The alpha-hydroperoxy radicals are assumed to decompose rapidly to OH and the carbonyl on the basis of estimated high exothermicity. Reaction at the 2- or 3-positions are estimated to occur no more than ~10% of the time and are neglected.
92	Reaction assumed to occur with the same rate and analogous mechanism as methyl hydroperoxide.
93	Absorption cross sections from Plum et al (1983), as recommended by IUPAC (Atkinson et al, 1997, 1999).
94	For the low wavelength band, a constant quantum yield of 0.4 is assumed, based on data of Langford and Moore (1984). For the high wavelength band, quantum yield is assumed to decrease linearly to zero at the threshold wavelength of 418 nm, starting at a "falloff" wavelength, which is adjusted to yield fits to chamber data for acetylene - NOx and acetylene reactivity experiments, as discussed by Carter et al (1997c). "Best fit" falloff wavelength of 380 nm used. Note that this gives overall quantum yields which are ~1.4 times higher than overall quantum yield reported by Plum et al (1983) for conditions of those experiments. Although use of acetylene reactivity data is a highly indirect way to obtain glyoxal quantum yields, it is considered to be a less uncertain way to estimate radical quantum yields then the data of Plum et al (1993), which uses a UV-poor light source and only measures rates of glyoxal decay.
95	Plum et al (1983) observed 13% formaldehyde yield in photodecomposition, so overall quantum yield adjusted to give this yield relative to the radical forming process for the spectral distribution of those experiments. A wavelength-independent quantum yield is used because of lack of information on wavelength dependence.
96	Product distribution based on the data of Niki et al (1985), as discussed by IUPAC (Atkinson et al, 1997). Product distribution is calculated for 1 atm air at 298K.
97	HCO(CO)OO. is represented by the lumped higher acyl peroxy species RCO-OO.

Table A-4 (continued)

No.	Note
98	The rate constant is estimated based on the correlation noted by Atkinson (1991) between HO and NO_3 radical H-atom abstraction rate constants, where the 298K H abstraction rate constants per abstractable hydrogen are approximately fit by $\ln k_{NO3} = 6.498 + 1.611 \ln k_{OH}$. The 298K rate constant is then derived from the 298K OH radical rate constant, assuming that all the reaction is at the OH group, and the temperature dependence is derived by assuming the same A factor per abstractable hydrogen as that for the reaction of NO_3 with acetaldehyde.
99	Absorption cross sections obtained from Moortgat (personal communication, 1996). These are essentially the same as those recommended by IUPAC (Atkinson et al, 1997, 1999), except slightly better resolution. Photolysis at the low wavelength band is assumed to have unit quantum yields, based on data for biacetyl. Photolysis above the cutoff wavelength of 421 nm (Atkinson et al, 1977a) is assumed to have zero quantum yields. For the rest of the high wavelength region, the wavelength dependence was derived by assuming the quantum yields decline linearly from 1 at 344 nm to 0 at a wavelength (407 nm) which was adjusted to be such that the calculated overall quantum yields for the conditions of the experiments of Plum et al (1983) agreed with the overall quantum yield they observed experimentally. The quantum yields recommended by IUPAC (Atkinson et al, 1999) lack sufficient wavelength resolution to be useful for modeling.
100	Absorption cross sections from Plum et al (1983). The evaluations give no recommendations for biacetyl.
101	Assumed to have unit quantum yield at low wavelength band based on data cited by Atkinson (1994). For the high wavelength band, the quantum yields were assumed to decline linearly from 1 at 350 nm to 0 at a wavelength (420 nm) which was adjusted to be such that the calculated overall quantum yields for the conditions of the experiments of Plum et al (1983) agreed with the overall quantum yield they observed experimentally.
102	Rate constant recommended by Atkinson (1994) for o-cresol.
103	The parameterized mechanism is estimated by analogy to the parameterized mechanism derived for cresols (see footnotes for OH + cresol reaction).
104	In absence of definitive data concerning this reaction, the same mechanism is used as assumed by Carter (1990). However, see footnotes concerning phenoxy reactions.
105	The parameterized mechanism is based on that used by Carter (1990), but was reoptimized to fit the NO, ozone, PAN, and cresol data in the o-cresol - NOx experiment EC281.
106	Assumed to have the same rate constant as the reaction of NO_3 with phenol. Reaction with NO_3 is assumed to dominate over reaction with OH radicals and other loss processes.
107	Absorption coefficients are from Majer et al (1969). The overall quantum yield derived by Carter (1990), which are based on model simulations of benzaldehyde decay rates in SAPRC evacuable chamber experiments, is used. Because of lack of data, the quantum yield is assumed to be independent of wavelength. The products formed from benzaldehyde photolysis are unknown, except that both radical formation and benzene formation appear to be minor (Carter, 1990). This benzaldehyde photolysis mechanism gives reasonably good model simulations of benzaldehyde - NOx experiments recently carried out in the CE-CERT xenon Teflon chamber (Carter et al, 1998a).
108	T=298K rate constant recommended by Atkinson (1994). Temperature dependence estimated by assuming the reaction has the same A factor as the reaction of NO_3 with acetaldehyde.
109	The rate constant and mechanism of Carter and Atkinson (1996) was used with no significant changes (except as indicated in other footnotes, if applicable). Some minor changes in product yields may result in some cases from use of the general mechanism estimation system to generate the overall reaction scheme.
110	MEK is used to represent hydroxyacetone.

Table A-4 (continued)

No.	Note
111	The excited $HCHO_2$ biradical is assumed to react as recommended by Atkinson (1997) based on data for the O3 + ethene system, i.e., 37% stabilization, 12% decomposition to HCO + OH, 13% decomposition to CO_2 + H_2, and 38% decomposition to CO + H_2O. Note that this is different than used for this species when formed in the isoprene products mechanisms of Carter and Atkinson (1996) and Carter (1996).
112	The vibrationally excited $HCOC(CH_3)CO_2$ biradicals are assumed to rearrange and decompose to $HCOC(O)CH_2$. + OH, where the former forms HCOC(O). + HCHO after O2 addition and NO to NO_2 conversion. RCO-O2. is used to represent HCOC(O)OO. in this reaction. Vibrationally excited $CH_3C(O)CHO_2$ is assumed to rapidly convert to $HCOC(CH_3)CO_2$ as discussed by Carter and Atkinson (1996).
113	The organic acid(s) formed in this reaction represent the formation of stabilizied Crigiee biradicals, which are assumed to be consumed primairly by reaction with H_2O forming the corresponding acid.
114	NO_3 radical addition assumed to occur primarily at the least substituted position.
115	The product CH3C(O)CH2ONO2 is expected to be relatively unreactive and is represented as "lost nitrogen" + 3 "lost carbons".
116	Rate constant estimated from linear correlation between log k for OH and O3P reaction. Chamber data for C_{3+} alkenes are better fit by models assuming O3P reactions with C_{3+} species do not form radicals. Stable products represented by the lumped higher aldehyde or ketone, depending on type of product(s) expected to be formed.
117	The overall quantum yield was reoptimized to fit the same data as discussed by Carter and Atkinson (1996). In the case of methacrolein, he changes to the other portion of the mechanism resulted in an ~14% increase in the best fit overall quantum yield compared to that derived by Carter and Atkinson (1996). In the case of MVK, the best fit overall quantum yield decreased by a factor of 5.
118	CH_2=CHC(O)OO. is represented by MA-RCO3.
119	As discussed by Carter (1996), ISOPROD is the "four product" lumped isoprene product species whose mechanism is derived by lumping rate constant and product parameters for a mixture of 30% hydroxymethacrolein, and 70% equal amounts of cis and trans $HCOC(CH_3)$=$CHCH_2OH$ and $HCOCH=C(CH_3)CH_2OH$. These proportions are based on the estimated yields of these products in the reactions of OH with isoprene (Carter and Atkinson, 1996), which are represented by ISOPROD in the four product condensed mechanism (Carter, 1996). The other footnotes refer to the estimated mechanisms for these four individual compounds which were used to derive the lumped ISOPROD mechanism. RCHO, PROD2, MA-RCO3, etc. are used to represent various compounds as indicated in the descriptions of these lumped model species. See Carter and Atkinson (1996) for the specific compounds which can be formed in the various reactions of these species.
120	The $HC(O)CHO_2$ biradical can decopose either to OH + HCO + CO via an internal H abstraction from HCO, or to HCO + HCO_2 via rearrangement to HCOCH(O.)O. and decomposition. (The HCO would form HO_2 + CO and the HCO_2 would form HO_2 + CO_2 after reaction with O_2.) These two pathways are assumed to have equal probability. Note that decomposition for these biradicals is assumed to be faster than for biradicals such as CH_3CHO_2 because of the weaker H-CO and C-CO bonds.

Table A-4 (continued)

No.	Note
121	The excited $CH_3C(O_2)CH_2OH$ biradical is assumed to react primarily via rearrangement to the unsaturated hydroperoxide followed by decomposition to OH radicals and the corresponding carbonyl compound, as is assumed in the general alkene mechanism. Two possible such rearrangements can occur in the case of this biradical, one to CH_2=C(OOH)CH_2OH, which decomposes to OH + $HOCH_2C(O)CH_2$., and the other to HOCH=C(OOH)CH_3, which decomposes to OH + $CH_3C(O)CH(.)OH$. The relative importances of the competing rearrangements in such cases is estimated by assuming they are approximately proportional to the estimated OH abstracting rate constant from the H-donating group. Based on this, the overall reaction is estimated to be OH + 0.04 $HOCH_2C(O)CH_2$. + 0.96 $CH_3C(O)CH(.)OH$, with the subsequent reactions of these radicals being derived by the general estimation methods.
122	All the species represented by ISOPROD are assumed to have the same overall photolysis rate as used for methacrolein.
123	The PROD2 mechanism was derived by averaging mechanisms for $CH_3C(O)CH_2CH_2CH_2OH$, $CH_3C(O)CH_2CH(CH_3)CH_2OH$, $CH_3CH(OH)CH_2CH_2C(O)CH_2CH_3$, $CH_3CH_2CH(OH)CH_2CH_2C(O)CH_2$-$CH_3$, and $CH_3CH_2CH_2CH(OH)CH_2CH_2C(O)CH_2CH_3$, which were taken as represent-ative of the products formed from VOCs measured in ambient air that are represented by PROD2 in the model (Carter, 1999). The mechanisms for these five representative PROD2 compounds were derived using the mechanism generation and estimation methods discussed in this report.
124	Assumed to photolyze with the same rate absorption cross section as used for MEK and other higher ketones. The overall quantum yield is assumed to be the same as that which gives best fits to chamber data for 2-heptanone (Carter et al, 2000e), which has the approximately the same number of carbons as the average for the set of compounds used to derive the PROD2 mechanism.
125	The RNO3 mechanism was derived by averaging mechanisms for $CH_3CH(ONO_2)CH_2CH_3$, $CH_3CH(OH)CH_2CH_2CH_2ONO_2$, $CH_3CH(ONO_2)CH(CH_3)CH_2CH_3$, $CH_3CH_2CH_2CH_2CH_2CH(ONO_2)CH_2$-OH, $CH_3CH(CH_3)CH_2C(CH_3)(ONO_2)CH_2CH_3$, and CH_3CH_2CH(ONO2)CH2CH_2-CH2-CH_2CH_2CH2CH_3, which were taken as representative of the products formed from VOCs measured in ambient air that are represented by RNO3 in the model. The mechanisms for these three representative RNO3 compounds were derived using the mechanism generation and estimation methods discussed in this report.
126	Absorption cross sections given by IUPAC (Atkinson et al, 1997, 1999) for isopropyl nitrate are used. As discussed by IUPAC (Atkinson et al, 1999), the quantum yield is expected to be near unity for formation of NO2.
127	DCB1 is used to represent aromatic ring fragmentation products that do not undergo signficant photodecomposition to radicals. Its mechanism is largely parameterized, but it is based roughly on that expected for unsaturated dicarbonys such as 2-butene-1,3-dial.
128	The rate constant is based on data of Bierbach et al (1994). The reaction is assumed to proceed via addition of OH to double bond, followed by decomposition of the alkoxy radical to HCO and HC(O)CH(OH)CHO, where the latter is represented by RCHO. Although this mechanism may not be what one would estimate for the non-photoreactive unsaturated diketones (Bierback et al, 1994; Tuazon et al, 1985) expected to be formed from o-substitued aromatics, best fits to the o-xylene and 1,2,4-trimethylbenzene chamber data are obtained if this mechanism is used.

Table A-4 (continued)

No.	Note

129 The photolysis action spectra of these products are assumed to be similar to that for acrolein, so the absorption cross sections of acrolein are used, with a wavelength-independent overall quantum yield. The overall quantum yield is adjusted to optimize fits of model simulations to the benzene - NOx experiments used in the optimization of the previous version of the mechanism by Carter et al (1997), The photolyisis mechanism is represented as being similar to that used for DCB2 and DCB3. However, best fits to benzene - NOx experiments are obtained if this photolysis is assumed to be slow, so the reaction is not included in the mechanism.

130 The rate constant is based on the data of Bierbach et al (1994). The reaction is assumed to involve initial formation of glyoxal and $HC(O)CHO_2$.

131 DCB2 and DCB3 represent the highly photoreactive unsaturated dicarbonyl product formed from the ring-opening reactions of the alkylbenzenes. To fit chamber data using differing light sources, they are represented by two species, which differ only in their action spectra and overall quantum yields, with the action spectrum of DCB2 being like methyl glyoxal, and that of DCB3 being like acrolein, and with the overall quantum yields adjusted separately to fit chamber data. Its reactions are based roughly on estimated reactions of a 5-carbon compound with general structure XC(O)CX=CXC(O)X, where X can be H or alkyl.

132 Assumed to have the same rate constant as used for DCB1. Mechanism represented as OH adding to double bond in XC(O)CX=CXC(O)X, with alkoxy radical decomposing to CH3CO. and XCO-CH(OH)-CXO, the latter being represented by RCHO. Note that the general alkoxy radical estimation method predicts that alkoxy radicals like RCH(OH)CH(O.)C(O)R' will decompose primarily to RCH(OH)CHO + RC(O).

133 The overall quantum yields for DCB2 and DCB3 were optimized to give best fits of model simulations of NO oxidation, O3 formation and xylene consumption in m-xylene - NOx chamber runs with various light sources, and also to mini-surrogate - NOx runs. The DCB2 and DCB3 quantum yields had to be adjusted as well as the yields of these products from m-xylene to best fit the data for the various light sources, and also to fit the results of the mini-surrogate as well as the m-xylene only runs. (For the other aromatics, only the DCB2 and DCB3 yields are optimized.) The photolysis mechanisms are unknown, and probably highly variable depending on the species involved. For an RC(O)CH=CHC(O)H structure, the most energetically favored initial reaction is formation of R. + HCOCH=CHCO., but assuming that mechanism results in a model that consistently underpredicts PAN yields in alkylbenzene - NOx chamber experiments. Therefore, a set of products is assumed to be formed that may result from various different reactions, and give predictions of PAN yields that are more consistent with available chamber data.

134 See discussion of mechanism generation system for documentation details for individual VOCs.

135 Based largely on "four product" isoprene mechanism of Carter (1996).

136 Mechanisms and rate parameters are emissions-weighed averages of those for the five terpenes with the highest estimated total annual North American emissions as given by Guenther et al (1999).

137 Mechanism for ethane, the only compound in this lumped class present in the base ROG mixture that is used to derive the mechanisms of these lumped species.

138 Mechanism based on 41% acetylene and 59% propane, the two compounds in this class present in the base ROG mixture that is used to derive the mechanisms for the lumped species. The ratio is based on the relative number of moles of each present in the mixture. The reaction of acetylene with O3 is ignored.

139 Mechanism and rate parameters are averages for the compounds in this class that are present in the base ROG mixture that is used to derive the mechanisms of these lumped species.

Table A-4 (continued)

No.	Note
140	Mechanism is the average for the compounds in this class that are present in the base ROG mixture that is used to derive the mechanisms of these lumped species. The rate parameters are those for toluene, the major compound in this class. The contribution of benzene to the mixture is given a reactivity weighting factor of 0.295, based on its kinetic reactivity [calculated using an IntOH of 110 ppt-min (Middleton et al, 1990)] relative to that of toluene.

Table A-5. Listing of the absorption cross sections and quantum yields for the photolysis reactions.

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
							NO2							
205.0	4.31e-19	1.000	210.0	4.72e-19	1.000	215.0	4.95e-19	1.000	220.0	4.56e-19	1.000	225.0	3.79e-19	1.000
230.0	2.74e-19	1.000	235.0	1.67e-19	1.000	240.0	9.31e-20	1.000	245.0	4.74e-20	1.000	250.0	2.48e-20	1.000
255.0	1.95e-20	1.000	260.0	2.24e-20	1.000	265.0	2.73e-20	1.000	270.0	4.11e-20	1.000	275.0	4.90e-20	1.000
280.0	5.92e-20	1.000	285.0	7.39e-20	1.000	290.0	9.00e-20	1.000	295.0	1.09e-19	1.000	300.0	1.31e-19	1.000
305.0	1.57e-19	1.000	310.0	1.86e-19	1.000	315.0	2.15e-19	0.990	320.0	2.48e-19	0.990	325.0	2.81e-19	0.990
330.0	3.13e-19	0.990	335.0	3.43e-19	0.990	340.0	3.80e-19	0.990	345.0	4.07e-19	0.990	350.0	4.31e-19	0.990
355.0	4.72e-19	0.990	360.0	4.83e-19	0.980	365.0	5.17e-19	0.980	370.0	5.32e-19	0.980	375.0	5.51e-19	0.980
380.0	5.64e-19	0.970	385.0	5.76e-19	0.970	390.0	5.93e-19	0.960	395.0	5.85e-19	0.935	400.0	6.02e-19	0.820
405.0	5.78e-19	0.355	410.0	6.00e-19	0.130	411.0	5.93e-19	0.110	412.0	5.86e-19	0.094	413.0	5.79e-19	0.083
414.0	5.72e-19	0.070	415.0	5.65e-19	0.059	416.0	5.68e-19	0.048	417.0	5.71e-19	0.039	418.0	5.75e-19	0.030
419.0	5.78e-19	0.023	420.0	5.81e-19	0.018	421.0	5.72e-19	0.012	422.0	5.64e-19	0.008	423.0	5.55e-19	0.004
424.0	5.47e-19	0.000												
							NO3NO							
585.0	2.89e-18	0.000	586.0	3.32e-18	0.050	587.0	4.16e-18	0.100	588.0	5.04e-18	0.150	589.0	6.13e-18	0.200
590.0	5.96e-18	0.250	591.0	5.44e-18	0.280	592.0	5.11e-18	0.310	593.0	4.58e-18	0.340	594.0	4.19e-18	0.370
595.0	4.29e-18	0.400	596.0	4.62e-18	0.370	597.0	4.36e-18	0.340	598.0	3.67e-18	0.310	599.0	3.10e-18	0.280
600.0	2.76e-18	0.250	601.0	2.86e-18	0.240	602.0	3.32e-18	0.230	603.0	3.80e-18	0.220	604.0	4.37e-18	0.210
605.0	4.36e-18	0.200	606.0	3.32e-18	0.200	607.0	2.40e-18	0.200	608.0	1.85e-18	0.200	609.0	1.71e-18	0.200
610.0	1.77e-18	0.200	611.0	1.91e-18	0.180	612.0	2.23e-18	0.160	613.0	2.63e-18	0.140	614.0	2.55e-18	0.120
615.0	2.26e-18	0.100	616.0	2.09e-18	0.100	617.0	2.11e-18	0.100	618.0	2.39e-18	0.100	619.0	2.56e-18	0.100
620.0	3.27e-18	0.100	621.0	5.24e-18	0.090	622.0	1.02e-17	0.080	623.0	1.47e-17	0.070	624.0	1.21e-17	0.060
625.0	8.38e-18	0.050	626.0	7.30e-18	0.050	627.0	7.53e-18	0.050	628.0	7.37e-18	0.050	629.0	6.98e-18	0.050
630.0	6.76e-18	0.050	631.0	4.84e-18	0.046	632.0	3.27e-18	0.042	633.0	2.17e-18	0.038	634.0	1.64e-18	0.034
635.0	1.44e-18	0.030	636.0	1.69e-18	0.024	637.0	2.07e-18	0.018	638.0	2.03e-18	0.012	639.0	1.58e-18	0.006
640.0	1.23e-18	0.000												
							NO3NO2							
400.0	0.00e+00	1.000	401.0	0.00e+00	1.000	402.0	0.00e+00	1.000	403.0	2.00e-20	1.000	404.0	0.00e+00	1.000
405.0	3.00e-20	1.000	406.0	2.00e-20	1.000	407.0	1.00e-20	1.000	408.0	3.00e-20	1.000	409.0	0.00e+00	1.000
410.0	1.00e-20	1.000	411.0	2.00e-20	1.000	412.0	5.00e-20	1.000	413.0	5.00e-20	1.000	414.0	2.00e-20	1.000
415.0	6.00e-20	1.000	416.0	6.00e-20	1.000	417.0	7.00e-20	1.000	418.0	5.00e-20	1.000	419.0	8.00e-20	1.000
420.0	8.00e-20	1.000	421.0	8.00e-20	1.000	422.0	9.00e-20	1.000	423.0	1.10e-19	1.000	424.0	9.00e-20	1.000
425.0	7.00e-20	1.000	426.0	1.40e-19	1.000	427.0	1.40e-19	1.000	428.0	1.20e-19	1.000	429.0	1.10e-19	1.000
430.0	1.70e-19	1.000	431.0	1.30e-19	1.000	432.0	1.50e-19	1.000	433.0	1.80e-19	1.000	434.0	1.80e-19	1.000
435.0	1.60e-19	1.000	436.0	1.50e-19	1.000	437.0	1.80e-19	1.000	438.0	2.10e-19	1.000	439.0	2.00e-19	1.000
440.0	1.90e-19	1.000	441.0	1.80e-19	1.000	442.0	2.10e-19	1.000	443.0	1.80e-19	1.000	444.0	1.90e-19	1.000
445.0	2.00e-19	1.000	446.0	2.40e-19	1.000	447.0	2.90e-19	1.000	448.0	2.40e-19	1.000	449.0	2.80e-19	1.000
450.0	2.90e-19	1.000	451.0	3.00e-19	1.000	452.0	3.30e-19	1.000	453.0	3.10e-19	1.000	454.0	3.60e-19	1.000
455.0	3.60e-19	1.000	456.0	3.60e-19	1.000	457.0	4.00e-19	1.000	458.0	3.70e-19	1.000	459.0	4.20e-19	1.000
460.0	4.00e-19	1.000	461.0	3.90e-19	1.000	462.0	4.00e-19	1.000	463.0	4.10e-19	1.000	464.0	4.80e-19	1.000
465.0	5.10e-19	1.000	466.0	5.40e-19	1.000	467.0	5.70e-19	1.000	468.0	5.60e-19	1.000	469.0	5.80e-19	1.000
470.0	5.90e-19	1.000	471.0	6.20e-19	1.000	472.0	6.40e-19	1.000	473.0	6.20e-19	1.000	474.0	6.20e-19	1.000
475.0	6.80e-19	1.000	476.0	7.80e-19	1.000	477.0	7.70e-19	1.000	478.0	7.30e-19	1.000	479.0	7.30e-19	1.000
480.0	7.00e-19	1.000	481.0	7.10e-19	1.000	482.0	7.10e-19	1.000	483.0	7.20e-19	1.000	484.0	7.70e-19	1.000
485.0	8.20e-19	1.000	486.0	9.10e-19	1.000	487.0	9.20e-19	1.000	488.0	9.50e-19	1.000	489.0	9.60e-19	1.000
490.0	1.03e-18	1.000	491.0	9.90e-19	1.000	492.0	9.90e-19	1.000	493.0	1.01e-18	1.000	494.0	1.01e-18	1.000
495.0	1.06e-18	1.000	496.0	1.21e-18	1.000	497.0	1.22e-18	1.000	498.0	1.20e-18	1.000	499.0	1.17e-18	1.000
500.0	1.13e-18	1.000	501.0	1.11e-18	1.000	502.0	1.11e-18	1.000	503.0	1.11e-18	1.000	504.0	1.26e-18	1.000
505.0	1.28e-18	1.000	506.0	1.34e-18	1.000	507.0	1.28e-18	1.000	508.0	1.27e-18	1.000	509.0	1.35e-18	1.000
510.0	1.51e-18	1.000	511.0	1.73e-18	1.000	512.0	1.77e-18	1.000	513.0	1.60e-18	1.000	514.0	1.58e-18	1.000
515.0	1.58e-18	1.000	516.0	1.56e-18	1.000	517.0	1.49e-18	1.000	518.0	1.44e-18	1.000	519.0	1.54e-18	1.000
520.0	1.68e-18	1.000	521.0	1.83e-18	1.000	522.0	1.93e-18	1.000	523.0	1.77e-18	1.000	524.0	1.64e-18	1.000
525.0	1.58e-18	1.000	526.0	1.63e-18	1.000	527.0	1.81e-18	1.000	528.0	2.10e-18	1.000	529.0	2.39e-18	1.000
530.0	2.23e-18	1.000	531.0	2.09e-18	1.000	532.0	2.02e-18	1.000	533.0	1.95e-18	1.000	534.0	2.04e-18	1.000
535.0	2.30e-18	1.000	536.0	2.57e-18	1.000	537.0	2.58e-18	1.000	538.0	2.34e-18	1.000	539.0	2.04e-18	1.000
540.0	2.10e-18	1.000	541.0	2.04e-18	1.000	542.0	1.88e-18	1.000	543.0	1.68e-18	1.000	544.0	1.70e-18	1.000
545.0	1.96e-18	1.000	546.0	2.42e-18	1.000	547.0	2.91e-18	1.000	548.0	2.98e-18	1.000	549.0	2.71e-18	1.000
550.0	2.48e-18	1.000	551.0	2.43e-18	1.000	552.0	2.47e-18	1.000	553.0	2.53e-18	1.000	554.0	2.78e-18	1.000
555.0	3.11e-18	1.000	556.0	3.26e-18	1.000	557.0	3.29e-18	1.000	558.0	3.51e-18	1.000	559.0	3.72e-18	1.000
560.0	3.32e-18	1.000	561.0	2.98e-18	1.000	562.0	2.90e-18	1.000	563.0	2.80e-18	1.000	564.0	2.72e-18	1.000
565.0	2.73e-18	1.000	566.0	2.85e-18	1.000	567.0	2.81e-18	1.000	568.0	2.85e-18	1.000	569.0	2.89e-18	1.000
570.0	2.79e-18	1.000	571.0	2.76e-18	1.000	572.0	2.74e-18	1.000	573.0	2.78e-18	1.000	574.0	2.86e-18	1.000
575.0	3.08e-18	1.000	576.0	3.27e-18	1.000	577.0	3.38e-18	1.000	578.0	3.31e-18	1.000	579.0	3.24e-18	1.000
580.0	3.34e-18	1.000	581.0	3.55e-18	1.000	582.0	3.28e-18	1.000	583.0	2.93e-18	1.000	584.0	2.82e-18	1.000
585.0	2.89e-18	1.000	586.0	3.32e-18	0.950	587.0	4.16e-18	0.900	588.0	5.04e-18	0.850	589.0	6.13e-18	0.800
590.0	5.96e-18	0.750	591.0	5.44e-18	0.720	592.0	5.11e-18	0.690	593.0	4.58e-18	0.660	594.0	4.19e-18	0.630
595.0	4.29e-18	0.600	596.0	4.62e-18	0.590	597.0	4.36e-18	0.580	598.0	3.67e-18	0.570	599.0	3.10e-18	0.560
600.0	2.76e-18	0.550	601.0	2.86e-18	0.540	602.0	3.32e-18	0.530	603.0	3.80e-18	0.520	604.0	4.37e-18	0.510
605.0	4.36e-18	0.400	606.0	3.32e-18	0.380	607.0	2.40e-18	0.360	608.0	1.85e-18	0.340	609.0	1.71e-18	0.320

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
610.0	1.77e-18	0.300	611.0	1.91e-18	0.290	612.0	2.23e-18	0.280	613.0	2.63e-18	0.270	614.0	2.55e-18	0.260
615.0	2.26e-18	0.250	616.0	2.09e-18	0.240	617.0	2.11e-18	0.230	618.0	2.39e-18	0.220	619.0	2.56e-18	0.210
620.0	3.27e-18	0.200	621.0	5.24e-18	0.190	622.0	1.02e-17	0.180	623.0	1.47e-17	0.170	624.0	1.21e-17	0.160
625.0	8.38e-18	0.150	626.0	7.30e-18	0.130	627.0	7.53e-18	0.110	628.0	7.37e-18	0.090	629.0	6.98e-18	0.070
630.0	6.76e-18	0.050	631.0	4.84e-18	0.040	632.0	3.27e-18	0.030	633.0	2.17e-18	0.020	634.0	1.64e-18	0.010
635.0	1.44e-18	0.000												
							O3O3P							
280.0	3.94e-18	0.095	281.0	3.62e-18	0.093	282.0	3.31e-18	0.090	283.0	2.99e-18	0.088	284.0	2.70e-18	0.086
285.0	2.46e-18	0.084	286.0	2.22e-18	0.082	287.0	1.98e-18	0.079	288.0	1.75e-18	0.077	289.0	1.59e-18	0.075
290.0	1.42e-18	0.073	291.0	1.25e-18	0.070	292.0	1.09e-18	0.068	293.0	9.81e-19	0.066	294.0	8.73e-19	0.064
295.0	7.65e-19	0.061	296.0	6.58e-19	0.059	297.0	5.81e-19	0.057	298.0	5.18e-19	0.055	299.0	4.55e-19	0.052
300.0	3.92e-19	0.050	301.0	3.35e-19	0.035	302.0	3.01e-19	0.025	303.0	2.66e-19	0.015	304.0	2.32e-19	0.010
305.0	1.97e-19	0.020	306.0	1.73e-19	0.050	307.0	1.55e-19	0.123	308.0	1.37e-19	0.227	309.0	1.18e-19	0.333
310.0	9.98e-20	0.400	311.0	8.92e-20	0.612	312.0	7.94e-20	0.697	313.0	6.96e-20	0.738	314.0	5.99e-20	0.762
315.0	5.01e-20	0.765	316.0	4.51e-20	0.779	317.0	4.00e-20	0.791	318.0	3.50e-20	0.806	319.0	2.99e-20	0.822
320.0	2.49e-20	0.852	321.0	2.23e-20	0.879	322.0	1.97e-20	0.903	323.0	1.72e-20	0.908	324.0	1.46e-20	0.920
325.0	1.20e-20	0.930	326.0	1.08e-20	0.934	327.0	9.67e-21	0.938	328.0	8.50e-21	0.942	329.0	7.34e-21	0.946
330.0	6.17e-21	0.950	331.0	5.48e-21	0.950	332.0	4.80e-21	0.950	333.0	4.11e-21	0.950	334.0	3.43e-21	0.950
335.0	2.74e-21	0.950	336.0	2.43e-21	0.960	337.0	2.11e-21	0.970	338.0	1.80e-21	0.980	339.0	1.48e-21	0.990
340.0	1.17e-21	1.000	350.0	0.00e+00	1.000	400.0	0.00e+00	1.000	410.0	1.20e-23	1.000	420.0	2.20e-23	1.000
440.0	1.12e-22	1.000	460.0	3.28e-22	1.000	480.0	6.84e-22	1.000	500.0	1.22e-21	1.000	520.0	1.82e-21	1.000
540.0	2.91e-21	1.000	560.0	3.94e-21	1.000	580.0	4.59e-21	1.000	600.0	5.11e-21	1.000	620.0	4.00e-21	1.000
640.0	2.96e-21	1.000	660.0	2.09e-21	1.000	680.0	1.36e-21	1.000	700.0	9.10e-22	1.000	750.0	3.20e-22	1.000
800.0	1.60e-22	1.000	900.0	0.00e+00	1.000									
							O3O1D							
280.0	3.94e-18	0.905	281.0	3.62e-18	0.907	282.0	3.31e-18	0.910	283.0	2.99e-18	0.912	284.0	2.70e-18	0.914
285.0	2.46e-18	0.916	286.0	2.22e-18	0.918	287.0	1.98e-18	0.921	288.0	1.75e-18	0.923	289.0	1.59e-18	0.925
290.0	1.42e-18	0.927	291.0	1.25e-18	0.930	292.0	1.09e-18	0.932	293.0	9.81e-19	0.934	294.0	8.73e-19	0.936
295.0	7.65e-19	0.939	296.0	6.58e-19	0.941	297.0	5.81e-19	0.943	298.0	5.18e-19	0.945	299.0	4.55e-19	0.948
300.0	3.92e-19	0.950	301.0	3.35e-19	0.965	302.0	3.01e-19	0.975	303.0	2.66e-19	0.985	304.0	2.32e-19	0.990
305.0	1.97e-19	0.980	306.0	1.73e-19	0.950	307.0	1.55e-19	0.877	308.0	1.37e-19	0.773	309.0	1.18e-19	0.667
310.0	9.98e-20	0.600	311.0	8.92e-20	0.388	312.0	7.94e-20	0.303	313.0	6.96e-20	0.262	314.0	5.99e-20	0.238
315.0	5.01e-20	0.235	316.0	4.51e-20	0.221	317.0	4.00e-20	0.209	318.0	3.50e-20	0.194	319.0	2.99e-20	0.178
320.0	2.49e-20	0.148	321.0	2.23e-20	0.121	322.0	1.97e-20	0.097	323.0	1.72e-20	0.092	324.0	1.46e-20	0.080
325.0	1.20e-20	0.070	326.0	1.08e-20	0.066	327.0	9.67e-21	0.062	328.0	8.50e-21	0.058	329.0	7.34e-21	0.054
330.0	6.17e-21	0.050	331.0	5.48e-21	0.050	332.0	4.80e-21	0.050	333.0	4.11e-21	0.050	334.0	3.43e-21	0.050
335.0	2.74e-21	0.050	336.0	2.43e-21	0.040	337.0	2.11e-21	0.030	338.0	1.80e-21	0.020	339.0	1.48e-21	0.010
340.0	1.17e-21	0.000												
							HONO-NO							
309.0	0.00e+00	0.410	310.0	1.30e-20	0.410	311.0	1.90e-20	0.411	312.0	2.80e-20	0.421	313.0	2.20e-20	0.432
314.0	3.60e-20	0.443	315.0	3.00e-20	0.454	316.0	1.40e-20	0.464	317.0	3.10e-20	0.475	318.0	5.60e-20	0.486
319.0	3.60e-20	0.496	320.0	4.90e-20	0.507	321.0	7.80e-20	0.518	322.0	4.90e-20	0.529	323.0	5.10e-20	0.539
324.0	7.10e-20	0.550	325.0	5.00e-20	0.561	326.0	2.90e-20	0.571	327.0	6.60e-20	0.582	328.0	1.17e-19	0.593
329.0	6.10e-20	0.604	330.0	1.11e-19	0.614	331.0	1.79e-19	0.625	332.0	8.70e-20	0.636	333.0	7.60e-20	0.646
334.0	9.60e-20	0.657	335.0	9.60e-20	0.668	336.0	7.20e-20	0.679	337.0	5.30e-20	0.689	338.0	1.00e-19	0.700
339.0	1.88e-19	0.711	340.0	1.00e-19	0.721	341.0	1.70e-19	0.732	342.0	3.86e-19	0.743	343.0	1.49e-19	0.754
344.0	9.70e-20	0.764	345.0	1.09e-19	0.775	346.0	1.23e-19	0.786	347.0	1.04e-19	0.796	348.0	9.10e-20	0.807
349.0	7.90e-20	0.818	350.0	1.12e-19	0.829	351.0	2.12e-19	0.839	352.0	1.55e-19	0.850	353.0	1.91e-19	0.861
354.0	5.81e-19	0.871	355.0	3.64e-19	0.882	356.0	1.41e-19	0.893	357.0	1.17e-19	0.904	358.0	1.20e-19	0.914
359.0	1.04e-19	0.925	360.0	9.00e-20	0.936	361.0	8.30e-20	0.946	362.0	8.00e-20	0.957	363.0	9.60e-20	0.968
364.0	1.46e-19	0.979	365.0	1.68e-19	0.989	366.0	1.83e-19	1.000	367.0	3.02e-19	1.000	368.0	5.20e-19	1.000
369.0	3.88e-19	1.000	370.0	1.78e-19	1.000	371.0	1.13e-19	1.000	372.0	1.00e-19	1.000	373.0	7.70e-20	1.000
374.0	6.20e-20	1.000	375.0	5.30e-20	1.000	376.0	5.30e-20	1.000	377.0	5.00e-20	1.000	378.0	5.80e-20	1.000
379.0	8.00e-20	1.000	380.0	9.60e-20	1.000	381.0	1.13e-19	1.000	382.0	1.59e-19	1.000	383.0	2.10e-19	1.000
384.0	2.41e-19	1.000	385.0	2.03e-19	1.000	386.0	1.34e-19	1.000	387.0	9.00e-20	1.000	388.0	5.60e-20	1.000
389.0	3.40e-20	1.000	390.0	2.70e-20	1.000	391.0	2.00e-20	1.000	392.0	1.50e-20	1.000	393.0	1.10e-20	1.000
394.0	6.00e-21	1.000	395.0	1.00e-20	1.000	396.0	4.00e-21	1.000	400.0	0.00e+00	1.000			
							HONO-NO2							
309.0	0.00e+00	0.590	310.0	1.30e-20	0.590	311.0	1.90e-20	0.589	312.0	2.80e-20	0.579	313.0	2.20e-20	0.568
314.0	3.60e-20	0.557	315.0	3.00e-20	0.546	316.0	1.40e-20	0.536	317.0	3.10e-20	0.525	318.0	5.60e-20	0.514
319.0	3.60e-20	0.504	320.0	4.90e-20	0.493	321.0	7.80e-20	0.482	322.0	4.90e-20	0.471	323.0	5.10e-20	0.461
324.0	7.10e-20	0.450	325.0	5.00e-20	0.439	326.0	2.90e-20	0.429	327.0	6.60e-20	0.418	328.0	1.17e-19	0.407
329.0	6.10e-20	0.396	330.0	1.11e-19	0.386	331.0	1.79e-19	0.375	332.0	8.70e-20	0.364	333.0	7.60e-20	0.354
334.0	9.60e-20	0.343	335.0	9.60e-20	0.332	336.0	7.20e-20	0.321	337.0	5.30e-20	0.311	338.0	1.00e-19	0.300
339.0	1.88e-19	0.289	340.0	1.00e-19	0.279	341.0	1.70e-19	0.268	342.0	3.86e-19	0.257	343.0	1.49e-19	0.246
344.0	9.70e-20	0.236	345.0	1.09e-19	0.225	346.0	1.23e-19	0.214	347.0	1.04e-19	0.204	348.0	9.10e-20	0.193
349.0	7.90e-20	0.182	350.0	1.12e-19	0.171	351.0	2.12e-19	0.161	352.0	1.55e-19	0.150	353.0	1.91e-19	0.139
354.0	5.81e-19	0.129	355.0	3.64e-19	0.118	356.0	1.41e-19	0.107	357.0	1.17e-19	0.096	358.0	1.20e-19	0.086
359.0	1.04e-19	0.075	360.0	9.00e-20	0.064	361.0	8.30e-20	0.054	362.0	8.00e-20	0.043	363.0	9.60e-20	0.032
364.0	1.46e-19	0.021	365.0	1.68e-19	0.011	366.0	1.83e-19	0.000						

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
							HNO3							
190.0	1.36e-17	1.000	195.0	1.02e-17	1.000	200.0	5.88e-18	1.000	205.0	2.80e-18	1.000	210.0	1.04e-18	1.000
215.0	3.65e-19	1.000	220.0	1.49e-19	1.000	225.0	8.81e-20	1.000	230.0	5.75e-20	1.000	235.0	3.75e-20	1.000
240.0	2.58e-20	1.000	245.0	2.11e-20	1.000	250.0	1.97e-20	1.000	255.0	1.95e-20	1.000	260.0	1.91e-20	1.000
265.0	1.80e-20	1.000	270.0	1.62e-20	1.000	275.0	1.38e-20	1.000	280.0	1.12e-20	1.000	285.0	8.58e-21	1.000
290.0	6.15e-21	1.000	295.0	4.12e-21	1.000	300.0	2.63e-21	1.000	305.0	1.50e-21	1.000	310.0	8.10e-22	1.000
315.0	4.10e-22	1.000	320.0	2.00e-22	1.000	325.0	9.50e-23	1.000	330.0	4.30e-23	1.000	335.0	2.20e-23	1.000
340.0	1.00e-23	1.000	345.0	6.00e-24	1.000	350.0	4.00e-24	1.000	355.0	0.00e+00	1.000			
							HO2NO2							
190.0	1.01e-17	1.000	195.0	8.16e-18	1.000	200.0	5.63e-18	1.000	205.0	3.67e-18	1.000	210.0	2.39e-18	1.000
215.0	1.61e-18	1.000	220.0	1.18e-18	1.000	225.0	9.32e-19	1.000	230.0	7.88e-19	1.000	235.0	6.80e-19	1.000
240.0	5.79e-19	1.000	245.0	4.97e-19	1.000	250.0	4.11e-19	1.000	255.0	3.49e-19	1.000	260.0	2.84e-19	1.000
265.0	2.29e-19	1.000	270.0	1.80e-19	1.000	275.0	1.33e-19	1.000	280.0	9.30e-20	1.000	285.0	6.20e-20	1.000
290.0	3.90e-20	1.000	295.0	2.40e-20	1.000	300.0	1.40e-20	1.000	305.0	8.50e-21	1.000	310.0	5.30e-21	1.000
315.0	3.90e-21	1.000	320.0	2.40e-21	1.000	325.0	1.50e-21	1.000	330.0	9.00e-22	1.000	335.0	0.00e+00	1.000
							H2O2							
190.0	6.72e-19	1.000	195.0	5.63e-19	1.000	200.0	4.75e-19	1.000	205.0	4.08e-19	1.000	210.0	3.57e-19	1.000
215.0	3.07e-19	1.000	220.0	2.58e-19	1.000	225.0	2.17e-19	1.000	230.0	1.82e-19	1.000	235.0	1.50e-19	1.000
240.0	1.24e-19	1.000	245.0	1.02e-19	1.000	250.0	8.30e-20	1.000	255.0	6.70e-20	1.000	260.0	5.30e-20	1.000
265.0	4.20e-20	1.000	270.0	3.30e-20	1.000	275.0	2.60e-20	1.000	280.0	2.00e-20	1.000	285.0	1.50e-20	1.000
290.0	1.20e-20	1.000	295.0	9.00e-21	1.000	300.0	6.80e-21	1.000	305.0	5.10e-21	1.000	310.0	3.90e-21	1.000
315.0	2.90e-21	1.000	320.0	2.20e-21	1.000	325.0	1.60e-21	1.000	330.0	1.30e-21	1.000	335.0	1.00e-21	1.000
340.0	7.00e-22	1.000	345.0	5.00e-22	1.000	350.0	4.00e-22	1.000	355.0	0.00e+00	1.000			
							HCHO_R							
240.0	6.40e-22	0.270	241.0	5.60e-22	0.272	242.0	1.05e-21	0.274	243.0	1.15e-21	0.276	244.0	8.20e-22	0.278
245.0	1.03e-21	0.280	246.0	9.80e-22	0.282	247.0	1.35e-21	0.284	248.0	1.91e-21	0.286	249.0	2.82e-21	0.288
250.0	2.05e-21	0.290	251.0	1.70e-21	0.291	252.0	2.88e-21	0.292	253.0	2.55e-21	0.293	254.0	2.55e-21	0.294
255.0	3.60e-21	0.295	256.0	5.09e-21	0.296	257.0	3.39e-21	0.297	258.0	2.26e-21	0.298	259.0	5.04e-21	0.299
260.0	5.05e-21	0.300	261.0	5.49e-21	0.308	262.0	5.20e-21	0.316	263.0	9.33e-21	0.324	264.0	8.23e-21	0.332
265.0	4.30e-21	0.340	266.0	4.95e-21	0.348	267.0	1.24e-20	0.356	268.0	1.11e-20	0.364	269.0	8.78e-21	0.372
270.0	9.36e-21	0.380	271.0	1.79e-20	0.399	272.0	1.23e-20	0.418	273.0	6.45e-21	0.437	274.0	6.56e-21	0.456
275.0	2.23e-20	0.475	276.0	2.42e-20	0.494	277.0	1.40e-20	0.513	278.0	1.05e-20	0.532	279.0	2.55e-20	0.551
280.0	2.08e-20	0.570	281.0	1.48e-20	0.586	282.0	8.81e-21	0.602	283.0	1.07e-20	0.618	284.0	4.49e-20	0.634
285.0	3.59e-20	0.650	286.0	1.96e-20	0.666	287.0	1.30e-20	0.682	288.0	3.36e-20	0.698	289.0	2.84e-20	0.714
290.0	1.30e-20	0.730	291.0	1.75e-20	0.735	292.0	8.32e-21	0.740	293.0	3.73e-20	0.745	294.0	6.54e-20	0.750
295.0	3.95e-20	0.755	296.0	2.33e-20	0.760	297.0	1.51e-20	0.765	298.0	4.04e-20	0.770	299.0	2.87e-20	0.775
300.0	8.71e-21	0.780	301.0	1.72e-20	0.780	302.0	1.06e-20	0.780	303.0	3.20e-20	0.780	304.0	6.90e-20	0.780
305.0	4.91e-20	0.780	306.0	4.63e-20	0.780	307.0	2.10e-20	0.780	308.0	1.49e-20	0.780	309.0	3.41e-20	0.780
310.0	1.95e-20	0.780	311.0	5.21e-21	0.764	312.0	1.12e-20	0.748	313.0	1.12e-20	0.732	314.0	4.75e-20	0.716
315.0	5.25e-20	0.700	316.0	2.90e-20	0.684	317.0	5.37e-20	0.668	318.0	2.98e-20	0.652	319.0	9.18e-21	0.636
320.0	1.26e-20	0.620	321.0	1.53e-20	0.585	322.0	6.69e-21	0.550	323.0	3.45e-21	0.515	324.0	8.16e-21	0.480
325.0	1.85e-20	0.445	326.0	5.95e-20	0.410	327.0	3.49e-20	0.375	328.0	1.09e-20	0.340	329.0	3.35e-20	0.305
330.0	3.32e-20	0.270	331.0	1.07e-20	0.243	332.0	2.89e-21	0.216	333.0	2.15e-21	0.189	334.0	1.71e-21	0.162
335.0	1.43e-21	0.135	336.0	1.94e-21	0.108	337.0	4.17e-21	0.081	338.0	2.36e-20	0.054	339.0	4.71e-20	0.027
340.0	2.48e-20	0.000												
							HCHO_M							
240.0	6.40e-22	0.490	241.0	5.60e-22	0.490	242.0	1.05e-21	0.490	243.0	1.15e-21	0.490	244.0	8.20e-22	0.490
245.0	1.03e-21	0.490	246.0	9.80e-22	0.490	247.0	1.35e-21	0.490	248.0	1.91e-21	0.490	249.0	2.82e-21	0.490
250.0	2.05e-21	0.490	251.0	1.70e-21	0.490	252.0	2.88e-21	0.490	253.0	2.55e-21	0.490	254.0	2.55e-21	0.490
255.0	3.60e-21	0.490	256.0	5.09e-21	0.490	257.0	3.39e-21	0.490	258.0	2.26e-21	0.490	259.0	5.04e-21	0.490
260.0	5.05e-21	0.490	261.0	5.49e-21	0.484	262.0	5.20e-21	0.478	263.0	9.33e-21	0.472	264.0	8.23e-21	0.466
265.0	4.30e-21	0.460	266.0	4.95e-21	0.454	267.0	1.24e-20	0.448	268.0	1.11e-20	0.442	269.0	8.78e-21	0.436
270.0	9.36e-21	0.430	271.0	1.79e-20	0.419	272.0	1.23e-20	0.408	273.0	6.45e-21	0.397	274.0	6.56e-21	0.386
275.0	2.23e-20	0.375	276.0	2.42e-20	0.364	277.0	1.40e-20	0.353	278.0	1.05e-20	0.342	279.0	2.55e-20	0.331
280.0	2.08e-20	0.320	281.0	1.48e-20	0.312	282.0	8.81e-21	0.304	283.0	1.07e-20	0.296	284.0	4.49e-20	0.288
285.0	3.59e-20	0.280	286.0	1.96e-20	0.272	287.0	1.30e-20	0.264	288.0	3.36e-20	0.256	289.0	2.84e-20	0.248
290.0	1.30e-20	0.240	291.0	1.75e-20	0.237	292.0	8.32e-21	0.234	293.0	3.73e-20	0.231	294.0	6.54e-20	0.228
295.0	3.95e-20	0.225	296.0	2.33e-20	0.222	297.0	1.51e-20	0.219	298.0	4.04e-20	0.216	299.0	2.87e-20	0.213
300.0	8.71e-21	0.210	301.0	1.72e-20	0.211	302.0	1.06e-20	0.212	303.0	3.20e-20	0.213	304.0	6.90e-20	0.214
305.0	4.91e-20	0.215	306.0	4.63e-20	0.216	307.0	2.10e-20	0.217	308.0	1.49e-20	0.218	309.0	3.41e-20	0.219
310.0	1.95e-20	0.220	311.0	5.21e-21	0.236	312.0	1.12e-20	0.252	313.0	1.12e-20	0.268	314.0	4.75e-20	0.284
315.0	5.25e-20	0.300	316.0	2.90e-20	0.316	317.0	5.37e-20	0.332	318.0	2.98e-20	0.348	319.0	9.18e-21	0.364
320.0	1.26e-20	0.380	321.0	1.53e-20	0.408	322.0	6.69e-21	0.436	323.0	3.45e-21	0.464	324.0	8.16e-21	0.492
325.0	1.85e-20	0.520	326.0	5.95e-20	0.548	327.0	3.49e-20	0.576	328.0	1.09e-20	0.604	329.0	3.35e-20	0.632
330.0	3.32e-20	0.660	331.0	1.07e-20	0.650	332.0	2.89e-21	0.640	333.0	2.15e-21	0.630	334.0	1.71e-21	0.620
335.0	1.43e-21	0.610	336.0	1.94e-21	0.600	337.0	4.17e-21	0.590	338.0	2.36e-20	0.580	339.0	4.71e-20	0.570
340.0	2.48e-20	0.560	341.0	7.59e-21	0.525	342.0	6.81e-21	0.490	343.0	1.95e-20	0.455	344.0	1.14e-20	0.420
345.0	3.23e-21	0.385	346.0	1.13e-21	0.350	347.0	6.60e-22	0.315	348.0	1.22e-21	0.280	349.0	3.20e-22	0.245
350.0	3.80e-22	0.210	351.0	1.04e-21	0.192	352.0	7.13e-21	0.174	353.0	2.21e-20	0.156	354.0	1.54e-20	0.138
355.0	6.76e-21	0.120	356.0	1.35e-21	0.102	357.0	3.60e-22	0.084	358.0	5.70e-23	0.066	359.0	5.80e-22	0.048
360.0	8.20e-22	0.000												

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
							CCHO_R							
262.0	2.44e-20	0.326	266.0	3.05e-20	0.358	270.0	3.42e-20	0.390	274.0	4.03e-20	0.466	278.0	4.19e-20	0.542
280.0	4.50e-20	0.580	281.0	4.69e-20	0.575	282.0	4.72e-20	0.570	283.0	4.75e-20	0.565	284.0	4.61e-20	0.560
285.0	4.49e-20	0.555	286.0	4.44e-20	0.550	287.0	4.59e-20	0.545	288.0	4.72e-20	0.540	289.0	4.77e-20	0.535
290.0	4.89e-20	0.530	291.0	4.78e-20	0.520	292.0	4.68e-20	0.510	293.0	4.53e-20	0.500	294.0	4.33e-20	0.490
295.0	4.27e-20	0.480	296.0	4.24e-20	0.470	297.0	4.38e-20	0.460	298.0	4.41e-20	0.450	299.0	4.26e-20	0.440
300.0	4.16e-20	0.430	301.0	3.99e-20	0.418	302.0	3.86e-20	0.406	303.0	3.72e-20	0.394	304.0	3.48e-20	0.382
305.0	3.42e-20	0.370	306.0	3.42e-20	0.354	307.0	3.36e-20	0.338	308.0	3.33e-20	0.322	309.0	3.14e-20	0.306
310.0	2.93e-20	0.290	311.0	2.76e-20	0.266	312.0	2.53e-20	0.242	313.0	2.47e-20	0.218	314.0	2.44e-20	0.194
315.0	2.20e-20	0.170	316.0	2.04e-20	0.156	317.0	2.07e-20	0.142	318.0	1.98e-20	0.128	319.0	1.87e-20	0.114
320.0	1.72e-20	0.100	321.0	1.48e-20	0.088	322.0	1.40e-20	0.076	323.0	1.24e-20	0.064	324.0	1.09e-20	0.052
325.0	1.14e-20	0.040	326.0	1.07e-20	0.032	327.0	8.58e-21	0.024	328.0	7.47e-21	0.016	329.0	7.07e-21	0.008
							C2CHO							
294.0	5.80e-20	0.890	295.0	5.57e-20	0.885	296.0	5.37e-20	0.880	297.0	5.16e-20	0.875	298.0	5.02e-20	0.870
299.0	5.02e-20	0.865	300.0	5.04e-20	0.860	301.0	5.09e-20	0.855	302.0	5.07e-20	0.850	303.0	4.94e-20	0.818
304.0	4.69e-20	0.786	305.0	4.32e-20	0.755	306.0	4.04e-20	0.723	307.0	3.81e-20	0.691	308.0	3.65e-20	0.659
309.0	3.62e-20	0.627	310.0	3.60e-20	0.596	311.0	3.53e-20	0.564	312.0	3.50e-20	0.532	313.0	3.32e-20	0.500
314.0	3.06e-20	0.480	315.0	2.77e-20	0.460	316.0	2.43e-20	0.440	317.0	2.18e-20	0.420	318.0	2.00e-20	0.400
319.0	1.86e-20	0.380	320.0	1.83e-20	0.360	321.0	1.78e-20	0.340	322.0	1.66e-20	0.320	323.0	1.58e-20	0.300
324.0	1.49e-20	0.280	325.0	1.30e-20	0.260	326.0	1.13e-20	0.248	327.0	9.96e-21	0.236	328.0	8.28e-21	0.223
329.0	6.85e-21	0.211	330.0	5.75e-21	0.199	331.0	4.94e-21	0.187	332.0	4.66e-21	0.174	333.0	4.30e-21	0.162
334.0	3.73e-21	0.150	335.0	3.25e-21	0.133	336.0	2.80e-21	0.117	337.0	2.30e-21	0.100	338.0	1.85e-21	0.083
339.0	1.66e-21	0.067	340.0	1.55e-21	0.050	341.0	1.19e-21	0.033	342.0	7.60e-22	0.017	343.0	4.50e-22	0.000
							ACETONE							
250.0	2.47e-20	0.760	254.0	3.04e-20	0.776	258.0	3.61e-20	0.792	262.0	4.15e-20	0.768	266.0	4.58e-20	0.704
270.0	4.91e-20	0.640	274.0	5.06e-20	0.604	278.0	5.07e-20	0.568	280.0	5.05e-20	0.550	281.0	5.01e-20	0.525
282.0	4.94e-20	0.500	283.0	4.86e-20	0.475	284.0	4.76e-20	0.450	285.0	4.68e-20	0.425	286.0	4.58e-20	0.400
287.0	4.50e-20	0.375	288.0	4.41e-20	0.350	289.0	4.29e-20	0.325	290.0	4.19e-20	0.302	291.0	4.08e-20	0.284
292.0	3.94e-20	0.266	293.0	3.81e-20	0.249	294.0	3.67e-20	0.232	295.0	3.52e-20	0.217	296.0	3.35e-20	0.201
297.0	3.20e-20	0.187	298.0	3.07e-20	0.173	299.0	2.91e-20	0.160	300.0	2.77e-20	0.147	301.0	2.66e-20	0.135
302.0	2.53e-20	0.124	303.0	2.37e-20	0.114	304.0	2.24e-20	0.104	305.0	2.11e-20	0.095	306.0	1.95e-20	0.086
307.0	1.80e-20	0.078	308.0	1.66e-20	0.071	309.0	1.54e-20	0.064	310.0	1.41e-20	0.057	311.0	1.28e-20	0.052
312.0	1.17e-20	0.046	313.0	1.08e-20	0.042	314.0	9.67e-21	0.037	315.0	8.58e-21	0.033	316.0	7.77e-21	0.029
317.0	6.99e-21	0.026	318.0	6.08e-21	0.023	319.0	5.30e-21	0.020	320.0	4.67e-21	0.018	321.0	4.07e-21	0.016
322.0	3.44e-21	0.014	323.0	2.87e-21	0.012	324.0	2.43e-21	0.011	325.0	2.05e-21	0.009	326.0	1.68e-21	0.008
327.0	1.35e-21	0.007	328.0	1.08e-21	0.006	329.0	8.60e-22	0.005	330.0	6.70e-22	0.005	331.0	5.10e-22	0.004
332.0	4.00e-22	0.003	333.0	3.10e-22	0.003	334.0	2.60e-22	0.002	335.0	1.70e-22	0.002	336.0	1.40e-22	0.002
337.0	1.10e-22	0.002	338.0	9.00e-23	0.001	339.0	6.00e-23	0.001	340.0	5.00e-23	0.001	341.0	5.00e-23	0.001
342.0	3.00e-23	0.001	343.0	4.00e-23	0.001	344.0	2.00e-23	0.000						
							KETONE							
198.5	3.95e-19	1.000	199.0	1.61e-19	1.000	199.5	7.75e-20	1.000	200.0	3.76e-20	1.000	200.5	2.51e-20	1.000
201.0	1.83e-20	1.000	201.5	1.36e-20	1.000	202.0	1.16e-20	1.000	202.5	8.97e-21	1.000	203.0	4.62e-21	1.000
203.5	3.18e-21	1.000	204.0	2.42e-21	1.000	204.5	2.01e-21	1.000	205.0	1.77e-21	1.000	205.5	1.64e-21	1.000
206.0	1.54e-21	1.000	206.5	1.52e-21	1.000	207.0	1.54e-21	1.000	207.5	1.62e-21	1.000	208.0	1.64e-21	1.000
208.5	1.60e-21	1.000	209.0	1.57e-21	1.000	209.5	1.49e-21	1.000	210.0	1.47e-21	1.000	210.5	1.52e-21	1.000
211.0	1.50e-21	1.000	211.5	1.62e-21	1.000	212.0	1.81e-21	1.000	212.5	2.10e-21	1.000	213.0	2.23e-21	1.000
213.5	2.06e-21	1.000	214.0	1.69e-21	1.000	214.5	1.49e-21	1.000	215.0	1.42e-21	1.000	215.5	1.42e-21	1.000
216.0	1.42e-21	1.000	216.5	1.48e-21	1.000	217.0	1.48e-21	1.000	217.5	1.53e-21	1.000	218.0	1.56e-21	1.000
218.5	1.67e-21	1.000	219.0	1.68e-21	1.000	219.5	1.78e-21	1.000	220.0	1.85e-21	1.000	220.5	1.92e-21	1.000
221.0	2.01e-21	1.000	221.5	2.11e-21	1.000	222.0	2.23e-21	1.000	222.5	2.33e-21	1.000	223.0	2.48e-21	1.000
223.5	2.60e-21	1.000	224.0	2.74e-21	1.000	224.5	2.85e-21	1.000	225.0	3.04e-21	1.000	225.5	3.15e-21	1.000
226.0	3.33e-21	1.000	226.5	3.55e-21	1.000	227.0	3.73e-21	1.000	227.5	3.93e-21	1.000	228.0	4.11e-21	1.000
228.5	4.34e-21	1.000	229.0	4.56e-21	1.000	229.5	4.75e-21	1.000	230.0	5.01e-21	1.000	230.5	5.27e-21	1.000
231.0	5.53e-21	1.000	231.5	5.83e-21	1.000	232.0	6.15e-21	1.000	232.5	6.45e-21	1.000	233.0	6.73e-21	1.000
233.5	7.02e-21	1.000	234.0	7.42e-21	1.000	234.5	7.83e-21	1.000	235.0	8.11e-21	1.000	235.5	8.45e-21	1.000
236.0	8.82e-21	1.000	236.5	9.21e-21	1.000	237.0	9.65e-21	1.000	237.5	1.00e-20	1.000	238.0	1.05e-20	1.000
238.5	1.10e-20	1.000	239.0	1.15e-20	1.000	239.5	1.20e-20	1.000	240.0	1.23e-20	1.000	240.5	1.28e-20	1.000
241.0	1.32e-20	1.000	241.5	1.38e-20	1.000	242.0	1.44e-20	1.000	242.5	1.50e-20	1.000	243.0	1.57e-20	1.000
243.5	1.63e-20	1.000	244.0	1.68e-20	1.000	244.5	1.75e-20	1.000	245.0	1.81e-20	1.000	245.5	1.88e-20	1.000
246.0	1.96e-20	1.000	246.5	2.03e-20	1.000	247.0	2.11e-20	1.000	247.5	2.19e-20	1.000	248.0	2.25e-20	1.000
248.5	2.33e-20	1.000	249.0	2.40e-20	1.000	249.5	2.48e-20	1.000	250.0	2.56e-20	1.000	250.5	2.64e-20	1.000
251.0	2.73e-20	1.000	251.5	2.81e-20	1.000	252.0	2.88e-20	1.000	252.5	2.98e-20	1.000	253.0	3.07e-20	1.000
253.5	3.16e-20	1.000	254.0	3.25e-20	1.000	254.5	3.34e-20	1.000	255.0	3.43e-20	1.000	255.5	3.51e-20	1.000
256.0	3.59e-20	1.000	256.5	3.67e-20	1.000	257.0	3.75e-20	1.000	257.5	3.84e-20	1.000	258.0	3.94e-20	1.000
258.5	4.03e-20	1.000	259.0	4.13e-20	1.000	259.5	4.22e-20	1.000	260.0	4.28e-20	1.000	260.5	4.33e-20	1.000
261.0	4.41e-20	1.000	261.5	4.49e-20	1.000	262.0	4.57e-20	1.000	262.5	4.65e-20	1.000	263.0	4.72e-20	1.000
263.5	4.78e-20	1.000	264.0	4.85e-20	1.000	264.5	4.92e-20	1.000	265.0	4.99e-20	1.000	265.5	5.04e-20	1.000
266.0	5.12e-20	1.000	266.5	5.22e-20	1.000	267.0	5.28e-20	1.000	267.5	5.34e-20	1.000	268.0	5.41e-20	1.000
268.5	5.46e-20	1.000	269.0	5.51e-20	1.000	269.5	5.55e-20	1.000	270.0	5.59e-20	1.000	270.5	5.63e-20	1.000
271.0	5.66e-20	1.000	271.5	5.70e-20	1.000	272.0	5.74e-20	1.000	272.5	5.78e-20	1.000	273.0	5.81e-20	1.000
273.5	5.86e-20	1.000	274.0	5.90e-20	1.000	274.5	5.93e-20	1.000	275.0	5.96e-20	1.000	275.5	5.97e-20	1.000
276.0	5.98e-20	1.000	276.5	5.98e-20	1.000	277.0	5.99e-20	1.000	277.5	5.99e-20	1.000	278.0	5.98e-20	1.000

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
278.5	5.96e-20	1.000	279.0	5.96e-20	1.000	279.5	5.95e-20	1.000	280.0	5.94e-20	1.000	280.5	5.92e-20	1.000
281.0	5.90e-20	1.000	281.5	5.88e-20	1.000	282.0	5.86e-20	1.000	282.5	5.83e-20	1.000	283.0	5.79e-20	1.000
283.5	5.75e-20	1.000	284.0	5.71e-20	1.000	284.5	5.67e-20	1.000	285.0	5.61e-20	1.000	285.5	5.56e-20	1.000
286.0	5.51e-20	1.000	286.5	5.45e-20	1.000	287.0	5.41e-20	1.000	287.5	5.37e-20	1.000	288.0	5.33e-20	1.000
288.5	5.27e-20	1.000	289.0	5.21e-20	1.000	289.5	5.15e-20	1.000	290.0	5.08e-20	1.000	290.5	4.99e-20	1.000
291.0	4.89e-20	1.000	291.5	4.82e-20	1.000	292.0	4.73e-20	1.000	292.5	4.62e-20	1.000	293.0	4.53e-20	1.000
293.5	4.41e-20	1.000	294.0	4.32e-20	1.000	294.5	4.23e-20	1.000	295.0	4.15e-20	1.000	295.5	4.11e-20	1.000
296.0	4.01e-20	1.000	296.5	3.94e-20	1.000	297.0	3.88e-20	1.000	297.5	3.77e-20	1.000	298.0	3.69e-20	1.000
298.5	3.63e-20	1.000	299.0	3.54e-20	1.000	299.5	3.46e-20	1.000	300.0	3.36e-20	1.000	300.5	3.24e-20	1.000
301.0	3.16e-20	1.000	301.5	3.06e-20	1.000	302.0	2.95e-20	1.000	302.5	2.82e-20	1.000	303.0	2.70e-20	1.000
303.5	2.59e-20	1.000	304.0	2.49e-20	1.000	304.5	2.42e-20	1.000	305.0	2.34e-20	1.000	305.5	2.28e-20	1.000
306.0	2.19e-20	1.000	306.5	2.11e-20	1.000	307.0	2.04e-20	1.000	307.5	1.93e-20	1.000	308.0	1.88e-20	1.000
308.5	1.80e-20	1.000	309.0	1.73e-20	1.000	309.5	1.66e-20	1.000	310.0	1.58e-20	1.000	310.5	1.48e-20	1.000
311.0	1.42e-20	1.000	311.5	1.34e-20	1.000	312.0	1.26e-20	1.000	312.5	1.17e-20	1.000	313.0	1.13e-20	1.000
313.5	1.08e-20	1.000	314.0	1.04e-20	1.000	314.5	9.69e-21	1.000	315.0	8.91e-21	1.000	315.5	8.61e-21	1.000
316.0	7.88e-21	1.000	316.5	7.25e-21	1.000	317.0	6.92e-21	1.000	317.5	6.43e-21	1.000	318.0	6.07e-21	1.000
318.5	5.64e-21	1.000	319.0	5.19e-21	1.000	319.5	4.66e-21	1.000	320.0	4.36e-21	1.000	320.5	3.95e-21	1.000
321.0	3.64e-21	1.000	321.5	3.38e-21	1.000	322.0	3.17e-21	1.000	322.5	2.80e-21	1.000	323.0	2.62e-21	1.000
323.5	2.29e-21	1.000	324.0	2.13e-21	1.000	324.5	1.93e-21	1.000	325.0	1.70e-21	1.000	325.5	1.58e-21	1.000
326.0	1.48e-21	1.000	326.5	1.24e-21	1.000	327.0	1.20e-21	1.000	327.5	1.04e-21	1.000	328.0	9.51e-22	1.000
328.5	8.44e-22	1.000	329.0	7.26e-22	1.000	329.5	6.70e-22	1.000	330.0	6.08e-22	1.000	330.5	5.15e-22	1.000
331.0	4.56e-22	1.000	331.5	4.13e-22	1.000	332.0	3.56e-22	1.000	332.5	3.30e-22	1.000	333.0	2.97e-22	1.000
333.5	2.67e-22	1.000	334.0	2.46e-22	1.000	334.5	2.21e-22	1.000	335.0	1.93e-22	1.000	335.5	1.56e-22	1.000
336.0	1.47e-22	1.000	336.5	1.37e-22	1.000	337.0	1.27e-22	1.000	337.5	1.19e-22	1.000	338.0	1.09e-22	1.000
338.5	1.01e-22	1.000	339.0	9.09e-23	1.000	339.5	8.22e-23	1.000	340.0	7.66e-23	1.000	340.5	7.43e-23	1.000
341.0	6.83e-23	1.000	341.5	6.72e-23	1.000	342.0	6.04e-23	1.000	342.5	4.78e-23	1.000	343.0	0.00e+00	1.000
COOH														
210.0	3.12e-19	1.000	215.0	2.09e-19	1.000	220.0	1.54e-19	1.000	225.0	1.22e-19	1.000	230.0	9.62e-20	1.000
235.0	7.61e-20	1.000	240.0	6.05e-20	1.000	245.0	4.88e-20	1.000	250.0	3.98e-20	1.000	255.0	3.23e-20	1.000
260.0	2.56e-20	1.000	265.0	2.11e-20	1.000	270.0	1.70e-20	1.000	275.0	1.39e-20	1.000	280.0	1.09e-20	1.000
285.0	8.63e-21	1.000	290.0	6.91e-21	1.000	295.0	5.51e-21	1.000	300.0	4.13e-21	1.000	305.0	3.13e-21	1.000
310.0	2.39e-21	1.000	315.0	1.82e-21	1.000	320.0	1.37e-21	1.000	325.0	1.05e-21	1.000	330.0	7.90e-22	1.000
335.0	6.10e-22	1.000	340.0	4.70e-22	1.000	345.0	3.50e-22	1.000	350.0	2.70e-22	1.000	355.0	2.10e-22	1.000
360.0	1.60e-22	1.000	365.0	1.20e-22	1.000	370.0	0.00e+00	1.000						
GLY_R														
230.0	2.87e-21	1.000	235.0	2.87e-21	1.000	240.0	4.30e-21	1.000	245.0	5.73e-21	1.000	250.0	8.60e-21	1.000
255.0	1.15e-20	1.000	260.0	1.43e-20	1.000	265.0	1.86e-20	1.000	270.0	2.29e-20	1.000	275.0	2.58e-20	1.000
280.0	2.87e-20	1.000	285.0	3.30e-20	1.000	290.0	3.15e-20	1.000	295.0	3.30e-20	1.000	300.0	3.58e-20	1.000
305.0	2.72e-20	1.000	310.0	2.72e-20	1.000	312.5	2.87e-20	1.000	315.0	2.29e-20	1.000	320.0	1.43e-20	1.000
325.0	1.15e-20	1.000	327.5	1.43e-20	1.000	330.0	1.15e-20	1.000	335.0	2.87e-21	1.000	340.0	0.00e+00	1.000
345.0	0.00e+00	1.000	350.0	0.00e+00	1.000	355.0	0.00e+00	1.000	360.0	2.29e-21	1.000	365.0	2.87e-21	1.000
370.0	8.03e-21	1.000	375.0	1.00e-20	1.000	380.0	1.72e-20	0.972	382.0	1.58e-20	0.855	384.0	1.49e-20	0.737
386.0	1.49e-20	0.619	388.0	2.87e-20	0.502	390.0	3.15e-20	0.384	391.0	3.24e-20	0.326	392.0	3.04e-20	0.267
393.0	2.23e-20	0.208	394.0	2.63e-20	0.149	395.0	3.04e-20	0.090	396.0	2.63e-20	0.032	397.0	2.43e-20	0.000
398.0	3.24e-20	0.000	399.0	3.04e-20	0.000	400.0	2.84e-20	0.000	401.0	3.24e-20	0.000	402.0	4.46e-20	0.000
403.0	5.27e-20	0.000	404.0	4.26e-20	0.000	405.0	3.04e-20	0.000	406.0	3.04e-20	0.000	407.0	2.84e-20	0.000
408.0	2.43e-20	0.000	409.0	2.84e-20	0.000	410.0	6.08e-20	0.000	411.0	5.07e-20	0.000	411.5	6.08e-20	0.000
412.0	4.86e-20	0.000	413.0	8.31e-20	0.000	413.5	6.48e-20	0.000	414.0	7.50e-20	0.000	414.5	8.11e-20	0.000
415.0	8.11e-20	0.000	415.5	6.89e-20	0.000	416.0	4.26e-20	0.000	417.0	4.86e-20	0.000	418.0	5.88e-20	0.000
GLY_ABS														
230.0	2.87e-21	1.000	235.0	2.87e-21	1.000	240.0	4.30e-21	1.000	245.0	5.73e-21	1.000	250.0	8.60e-21	1.000
255.0	1.15e-20	1.000	260.0	1.43e-20	1.000	265.0	1.86e-20	1.000	270.0	2.29e-20	1.000	275.0	2.58e-20	1.000
280.0	2.87e-20	1.000	285.0	3.30e-20	1.000	290.0	3.15e-20	1.000	295.0	3.30e-20	1.000	300.0	3.58e-20	1.000
305.0	2.72e-20	1.000	310.0	2.72e-20	1.000	312.5	2.87e-20	1.000	315.0	2.29e-20	1.000	320.0	1.43e-20	1.000
325.0	1.15e-20	1.000	327.5	1.43e-20	1.000	330.0	1.15e-20	1.000	335.0	2.87e-21	1.000	340.0	0.00e+00	1.000
355.0	0.00e+00	1.000	360.0	2.29e-21	1.000	365.0	2.87e-21	1.000	370.0	8.03e-21	1.000	375.0	1.00e-20	1.000
380.0	1.72e-20	1.000	382.0	1.58e-20	1.000	384.0	1.49e-20	1.000	386.0	1.49e-20	1.000	388.0	2.87e-20	1.000
390.0	3.15e-20	1.000	391.0	3.24e-20	1.000	392.0	3.04e-20	1.000	393.0	2.23e-20	1.000	394.0	2.63e-20	1.000
395.0	3.04e-20	1.000	396.0	2.63e-20	1.000	397.0	2.43e-20	1.000	398.0	3.24e-20	1.000	399.0	3.04e-20	1.000
400.0	2.84e-20	1.000	401.0	3.24e-20	1.000	402.0	4.46e-20	1.000	403.0	5.27e-20	1.000	404.0	4.26e-20	1.000
405.0	3.04e-20	1.000	406.0	3.04e-20	1.000	407.0	2.84e-20	1.000	408.0	2.43e-20	1.000	409.0	2.84e-20	1.000
410.0	6.08e-20	1.000	411.0	5.07e-20	1.000	411.5	6.08e-20	1.000	412.0	4.86e-20	1.000	413.0	8.31e-20	1.000
413.5	6.48e-20	1.000	414.0	7.50e-20	1.000	414.5	8.11e-20	1.000	415.0	8.11e-20	1.000	415.5	6.89e-20	1.000
416.0	4.26e-20	1.000	417.0	4.86e-20	1.000	418.0	5.88e-20	1.000	419.0	6.69e-20	1.000	420.0	3.85e-20	1.000
421.0	5.67e-20	1.000	421.5	4.46e-20	1.000	422.0	5.27e-20	1.000	422.5	1.05e-19	1.000	423.0	8.51e-20	1.000
424.0	6.08e-20	1.000	425.0	7.29e-20	1.000	426.0	1.18e-19	1.000	426.5	1.30e-19	1.000	427.0	1.07e-19	1.000
428.0	1.66e-19	1.000	429.0	4.05e-20	1.000	430.0	5.07e-20	1.000	431.0	4.86e-20	1.000	432.0	4.05e-20	1.000
433.0	3.65e-20	1.000	434.0	4.05e-20	1.000	434.5	6.08e-20	1.000	435.0	5.07e-20	1.000	436.0	8.11e-20	1.000
436.5	1.13e-19	1.000	437.0	5.27e-20	1.000	438.0	1.01e-19	1.000	438.5	1.38e-19	1.000	439.0	7.70e-20	1.000
440.0	2.47e-19	1.000	441.0	8.11e-20	1.000	442.0	6.08e-20	1.000	443.0	7.50e-20	1.000	444.0	9.32e-20	1.000
445.0	1.13e-19	1.000	446.0	5.27e-20	1.000	447.0	2.43e-20	1.000	448.0	2.84e-20	1.000	449.0	3.85e-20	1.000
450.0	6.08e-20	1.000	451.0	1.09e-19	1.000	451.5	9.32e-20	1.000	452.0	1.22e-19	1.000	453.0	2.39e-19	1.000

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
454.0	1.70e-19	1.000	455.0	3.40e-19	1.000	455.5	4.05e-19	1.000	456.0	1.01e-19	1.000	457.0	1.62e-20	1.000
458.0	1.22e-20	1.000	458.5	1.42e-20	1.000	459.0	4.05e-21	1.000	460.0	4.05e-21	1.000	460.5	6.08e-21	1.000
461.0	2.03e-21	1.000	462.0	0.00e+00	1.000									
						MGLY_ADJ								
219.0	9.84e-21	1.000	219.5	1.04e-20	1.000	220.0	1.06e-20	1.000	220.5	1.11e-20	1.000	221.0	1.15e-20	1.000
221.5	1.18e-20	1.000	222.0	1.22e-20	1.000	222.5	1.24e-20	1.000	223.0	1.26e-20	1.000	223.5	1.26e-20	1.000
224.0	1.25e-20	1.000	224.5	1.24e-20	1.000	225.0	1.25e-20	1.000	225.5	1.27e-20	1.000	226.0	1.27e-20	1.000
226.5	1.29e-20	1.000	227.0	1.31e-20	1.000	227.5	1.32e-20	1.000	228.0	1.35e-20	1.000	228.5	1.37e-20	1.000
229.0	1.40e-20	1.000	229.5	1.42e-20	1.000	230.0	1.48e-20	1.000	230.5	1.53e-20	1.000	231.0	1.57e-20	1.000
231.5	1.59e-20	1.000	232.0	1.61e-20	1.000	232.5	1.62e-20	1.000	233.0	1.61e-20	1.000	233.5	1.68e-20	1.000
234.0	1.74e-20	1.000	234.5	1.80e-20	1.000	235.0	1.84e-20	1.000	235.5	1.87e-20	1.000	236.0	1.89e-20	1.000
236.5	1.91e-20	1.000	237.0	1.93e-20	1.000	237.5	1.94e-20	1.000	238.0	1.96e-20	1.000	238.5	1.96e-20	1.000
239.0	2.01e-20	1.000	239.5	2.04e-20	1.000	240.0	2.08e-20	1.000	240.5	2.10e-20	1.000	241.0	2.14e-20	1.000
241.5	2.16e-20	1.000	242.0	2.19e-20	1.000	242.5	2.20e-20	1.000	243.0	2.23e-20	1.000	243.5	2.26e-20	1.000
244.0	2.28e-20	1.000	244.5	2.29e-20	1.000	245.0	2.30e-20	1.000	245.5	2.32e-20	1.000	246.0	2.33e-20	1.000
246.5	2.35e-20	1.000	247.0	2.38e-20	1.000	247.5	2.41e-20	1.000	248.0	2.46e-20	1.000	248.5	2.51e-20	1.000
249.0	2.57e-20	1.000	249.5	2.61e-20	1.000	250.0	2.65e-20	1.000	250.5	2.67e-20	1.000	251.0	2.69e-20	1.000
251.5	2.69e-20	1.000	252.0	2.71e-20	1.000	252.5	2.72e-20	1.000	253.0	2.73e-20	1.000	253.5	2.74e-20	1.000
254.0	2.76e-20	1.000	254.5	2.78e-20	1.000	255.0	2.82e-20	1.000	255.5	2.87e-20	1.000	256.0	2.93e-20	1.000
256.5	2.98e-20	1.000	257.0	3.07e-20	1.000	257.5	3.12e-20	1.000	258.0	3.17e-20	1.000	258.5	3.21e-20	1.000
259.0	3.26e-20	1.000	259.5	3.28e-20	1.000	260.0	3.29e-20	1.000	260.5	3.31e-20	1.000	261.0	3.33e-20	1.000
261.5	3.34e-20	1.000	262.0	3.36e-20	1.000	262.5	3.38e-20	1.000	263.0	3.42e-20	1.000	263.5	3.44e-20	1.000
264.0	3.48e-20	1.000	264.5	3.54e-20	1.000	265.0	3.59e-20	1.000	265.5	3.65e-20	1.000	266.0	3.73e-20	1.000
266.5	3.80e-20	1.000	267.0	3.87e-20	1.000	267.5	3.95e-20	1.000	268.0	4.02e-20	1.000	268.5	4.08e-20	1.000
269.0	4.13e-20	1.000	269.5	4.17e-20	1.000	270.0	4.20e-20	1.000	270.5	4.22e-20	1.000	271.0	4.22e-20	1.000
271.5	4.22e-20	1.000	272.0	4.23e-20	1.000	272.5	4.24e-20	1.000	273.0	4.27e-20	1.000	273.5	4.29e-20	1.000
274.0	4.31e-20	1.000	274.5	4.33e-20	1.000	275.0	4.37e-20	1.000	275.5	4.42e-20	1.000	276.0	4.48e-20	1.000
276.5	4.56e-20	1.000	277.0	4.64e-20	1.000	277.5	4.71e-20	1.000	278.0	4.78e-20	1.000	278.5	4.83e-20	1.000
279.0	4.87e-20	1.000	279.5	4.90e-20	1.000	280.0	4.92e-20	1.000	280.5	4.93e-20	1.000	281.0	4.94e-20	1.000
281.5	4.92e-20	1.000	282.0	4.90e-20	1.000	282.5	4.86e-20	1.000	283.0	4.83e-20	1.000	283.5	4.79e-20	1.000
284.0	4.76e-20	1.000	284.5	4.72e-20	1.000	285.0	4.70e-20	1.000	285.5	4.68e-20	1.000	286.0	4.66e-20	1.000
286.5	4.65e-20	1.000	287.0	4.65e-20	1.000	287.5	4.68e-20	1.000	288.0	4.73e-20	1.000	288.5	4.78e-20	1.000
289.0	4.84e-20	1.000	289.5	4.89e-20	1.000	290.0	4.92e-20	1.000	290.5	4.92e-20	1.000	291.0	4.90e-20	1.000
291.5	4.86e-20	1.000	292.0	4.81e-20	1.000	292.5	4.75e-20	1.000	293.0	4.70e-20	1.000	293.5	4.65e-20	1.000
294.0	4.58e-20	1.000	294.5	4.48e-20	1.000	295.0	4.38e-20	1.000	295.5	4.27e-20	1.000	296.0	4.17e-20	1.000
296.5	4.07e-20	1.000	297.0	3.99e-20	1.000	297.5	3.94e-20	1.000	298.0	3.88e-20	1.000	298.5	3.82e-20	1.000
299.0	3.76e-20	1.000	299.5	3.72e-20	1.000	300.0	3.69e-20	1.000	300.5	3.68e-20	1.000	301.0	3.70e-20	1.000
301.5	3.72e-20	1.000	302.0	3.74e-20	1.000	302.5	3.74e-20	1.000	303.0	3.75e-20	1.000	303.5	3.71e-20	1.000
304.0	3.62e-20	1.000	304.5	3.51e-20	1.000	305.0	3.38e-20	1.000	305.5	3.25e-20	1.000	306.0	3.15e-20	1.000
306.5	3.04e-20	1.000	307.0	2.92e-20	1.000	307.5	2.80e-20	1.000	308.0	2.71e-20	1.000	308.5	2.63e-20	1.000
309.0	2.52e-20	1.000	309.5	2.43e-20	1.000	310.0	2.34e-20	1.000	310.5	2.25e-20	1.000	311.0	2.19e-20	1.000
311.5	2.12e-20	1.000	312.0	2.06e-20	1.000	312.5	2.02e-20	1.000	313.0	1.96e-20	1.000	313.5	1.92e-20	1.000
314.0	1.91e-20	1.000	314.5	1.88e-20	1.000	315.0	1.86e-20	1.000	315.5	1.85e-20	1.000	316.0	1.86e-20	1.000
316.5	1.87e-20	1.000	317.0	1.87e-20	1.000	317.5	1.87e-20	1.000	318.0	1.83e-20	1.000	318.5	1.75e-20	1.000
319.0	1.69e-20	1.000	319.5	1.60e-20	1.000	320.0	1.50e-20	1.000	320.5	1.41e-20	1.000	321.0	1.34e-20	1.000
321.5	1.27e-20	1.000	322.0	1.21e-20	1.000	322.5	1.18e-20	1.000	323.0	1.14e-20	1.000	323.5	1.08e-20	1.000
324.0	1.01e-20	1.000	324.5	9.62e-21	1.000	325.0	9.28e-21	1.000	325.5	8.75e-21	1.000	326.0	8.49e-21	1.000
326.5	8.21e-21	1.000	327.0	7.71e-21	1.000	327.5	7.38e-21	1.000	328.0	7.18e-21	1.000	328.5	6.86e-21	1.000
329.0	6.71e-21	1.000	329.5	6.63e-21	1.000	330.0	6.46e-21	1.000	330.5	6.29e-21	1.000	331.0	6.21e-21	1.000
331.5	6.18e-21	1.000	332.0	6.20e-21	1.000	332.5	5.49e-21	1.000	333.0	5.21e-21	1.000	333.5	5.38e-21	1.000
334.0	5.35e-21	1.000	334.5	5.04e-21	1.000	335.0	4.94e-21	1.000	335.5	4.90e-21	1.000	336.0	4.52e-21	1.000
336.5	4.26e-21	1.000	337.0	4.11e-21	1.000	337.5	3.76e-21	1.000	338.0	3.61e-21	1.000	338.5	3.58e-21	1.000
339.0	3.47e-21	1.000	339.5	3.32e-21	1.000	340.0	3.22e-21	1.000	340.5	3.10e-21	1.000	341.0	3.00e-21	1.000
341.5	2.94e-21	1.000	342.0	2.89e-21	1.000	342.5	2.86e-21	1.000	343.0	2.88e-21	1.000	343.5	2.88e-21	1.000
344.0	2.89e-21	0.992	344.5	2.91e-21	0.984	345.0	2.95e-21	0.976	345.5	3.00e-21	0.968	346.0	3.08e-21	0.960
346.5	3.18e-21	0.953	347.0	3.25e-21	0.945	347.5	3.30e-21	0.937	348.0	3.39e-21	0.929	348.5	3.51e-21	0.921
349.0	3.63e-21	0.913	349.5	3.73e-21	0.905	350.0	3.85e-21	0.897	350.5	3.99e-21	0.889	351.0	4.27e-21	0.881
351.5	4.47e-21	0.873	352.0	4.63e-21	0.865	352.5	4.78e-21	0.858	353.0	4.92e-21	0.850	353.5	5.07e-21	0.842
354.0	5.23e-21	0.834	354.5	5.39e-21	0.826	355.0	5.56e-21	0.818	355.5	5.77e-21	0.810	356.0	5.97e-21	0.802
356.5	6.15e-21	0.794	357.0	6.35e-21	0.786	357.5	6.56e-21	0.778	358.0	6.76e-21	0.770	358.5	6.95e-21	0.763
359.0	7.20e-21	0.755	359.5	7.44e-21	0.747	360.0	7.64e-21	0.739	360.5	7.89e-21	0.731	361.0	8.15e-21	0.723
361.5	8.43e-21	0.715	362.0	8.71e-21	0.707	362.5	9.02e-21	0.699	363.0	9.33e-21	0.691	363.5	9.65e-21	0.683
364.0	1.00e-20	0.675	364.5	1.04e-20	0.668	365.0	1.08e-20	0.660	365.5	1.11e-20	0.652	366.0	1.15e-20	0.644
366.5	1.19e-20	0.636	367.0	1.23e-20	0.628	367.5	1.27e-20	0.620	368.0	1.31e-20	0.612	368.5	1.35e-20	0.604
369.0	1.40e-20	0.596	369.5	1.44e-20	0.588	370.0	1.47e-20	0.580	370.5	1.51e-20	0.573	371.0	1.55e-20	0.565
371.5	1.59e-20	0.557	372.0	1.64e-20	0.549	372.5	1.70e-20	0.541	373.0	1.73e-20	0.533	373.5	1.77e-20	0.525
374.0	1.81e-20	0.517	374.5	1.86e-20	0.509	375.0	1.90e-20	0.501	375.5	1.96e-20	0.493	376.0	2.02e-20	0.486
376.5	2.06e-20	0.478	377.0	2.10e-20	0.470	377.5	2.14e-20	0.462	378.0	2.18e-20	0.454	378.5	2.24e-20	0.446
379.0	2.30e-20	0.438	379.5	2.37e-20	0.430	380.0	2.42e-20	0.422	380.5	2.47e-20	0.414	381.0	2.54e-20	0.406
381.5	2.62e-20	0.398	382.0	2.69e-20	0.391	382.5	2.79e-20	0.383	383.0	2.88e-20	0.375	383.5	2.96e-20	0.367
384.0	3.02e-20	0.359	384.5	3.10e-20	0.351	385.0	3.20e-20	0.343	385.5	3.29e-20	0.335	386.0	3.39e-20	0.327
386.5	3.51e-20	0.319	387.0	3.62e-20	0.311	387.5	3.69e-20	0.303	388.0	3.70e-20	0.296	388.5	3.77e-20	0.288
389.0	3.88e-20	0.280	389.5	3.97e-20	0.272	390.0	4.03e-20	0.264	390.5	4.12e-20	0.256	391.0	4.22e-20	0.248

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
391.5	4.29e-20	0.240	392.0	4.30e-20	0.232	392.5	4.38e-20	0.224	393.0	4.47e-20	0.216	393.5	4.55e-20	0.208
394.0	4.56e-20	0.201	394.5	4.59e-20	0.193	395.0	4.67e-20	0.185	395.5	4.80e-20	0.177	396.0	4.87e-20	0.169
396.5	4.96e-20	0.161	397.0	5.08e-20	0.153	397.5	5.19e-20	0.145	398.0	5.23e-20	0.137	398.5	5.39e-20	0.129
399.0	5.46e-20	0.121	399.5	5.54e-20	0.113	400.0	5.59e-20	0.106	400.5	5.77e-20	0.098	401.0	5.91e-20	0.090
401.5	5.99e-20	0.082	402.0	6.06e-20	0.074	402.5	6.20e-20	0.066	403.0	6.35e-20	0.058	403.5	6.52e-20	0.050
404.0	6.54e-20	0.042	404.5	6.64e-20	0.034	405.0	6.93e-20	0.026	405.5	7.15e-20	0.018	406.0	7.19e-20	0.011
406.5	7.32e-20	0.003	407.0	7.58e-20	0.000	407.5	7.88e-20	0.000	408.0	7.97e-20	0.000	408.5	7.91e-20	0.000
409.0	8.11e-20	0.000	409.5	8.41e-20	0.000	410.0	8.53e-20	0.000	410.5	8.59e-20	0.000	411.0	8.60e-20	0.000
411.5	8.80e-20	0.000	412.0	9.04e-20	0.000	412.5	9.45e-20	0.000	413.0	9.34e-20	0.000	413.5	9.37e-20	0.000
414.0	9.63e-20	0.000	414.5	9.71e-20	0.000	415.0	9.70e-20	0.000	415.5	9.65e-20	0.000	416.0	9.69e-20	0.000
416.5	9.89e-20	0.000	417.0	1.00e-19	0.000	417.5	1.02e-19	0.000	418.0	1.00e-19	0.000	418.5	1.02e-19	0.000
419.0	1.01e-19	0.000	419.5	1.01e-19	0.000	420.0	1.03e-19	0.000	420.5	1.01e-19	0.000	421.0	1.04e-19	0.000
BACL_ADJ														
230.0	1.30e-20	1.000	232.5	1.46e-20	1.000	235.0	1.68e-20	1.000	237.5	1.84e-20	1.000	240.0	2.16e-20	1.000
242.5	2.49e-20	1.000	245.0	2.65e-20	1.000	247.5	2.71e-20	1.000	250.0	3.03e-20	1.000	252.5	3.46e-20	1.000
255.0	3.46e-20	1.000	257.5	3.57e-20	1.000	260.0	3.95e-20	1.000	262.5	4.17e-20	1.000	265.0	4.17e-20	1.000
267.5	4.22e-20	1.000	270.0	4.60e-20	1.000	272.5	4.54e-20	1.000	275.0	4.33e-20	1.000	277.5	4.22e-20	1.000
280.0	4.44e-20	1.000	282.5	4.33e-20	1.000	285.0	3.90e-20	1.000	287.5	3.57e-20	1.000	290.0	3.25e-20	1.000
292.5	2.92e-20	1.000	295.0	2.60e-20	1.000	297.5	2.16e-20	1.000	300.0	1.79e-20	1.000	302.5	1.73e-20	1.000
305.0	1.46e-20	1.000	307.5	1.08e-20	1.000	310.0	9.20e-21	1.000	312.5	7.03e-21	1.000	315.0	6.49e-21	1.000
317.5	5.41e-21	1.000	320.0	5.41e-21	1.000	322.5	5.41e-21	1.000	325.0	4.33e-21	1.000	327.5	3.25e-21	1.000
330.0	3.79e-21	1.000	332.5	3.79e-21	1.000	335.0	4.33e-21	1.000	337.5	4.87e-21	1.000	340.0	5.41e-21	1.000
342.5	5.95e-21	1.000	345.0	6.49e-21	1.000	347.5	7.03e-21	1.000	350.0	8.12e-21	0.995	352.5	7.57e-21	0.960
355.0	9.20e-21	0.925	357.5	9.74e-21	0.890	360.0	1.08e-20	0.855	362.5	1.19e-20	0.820	365.0	1.41e-20	0.785
367.5	1.51e-20	0.750	370.0	1.79e-20	0.715	372.5	2.00e-20	0.680	375.0	2.11e-20	0.645	377.5	2.33e-20	0.610
380.0	2.60e-20	0.575	382.5	2.81e-20	0.540	385.0	3.14e-20	0.505	387.5	3.46e-20	0.470	390.0	3.90e-20	0.435
392.5	4.11e-20	0.399	395.0	4.33e-20	0.364	397.5	4.38e-20	0.329	400.0	4.65e-20	0.294	402.5	4.81e-20	0.259
405.0	5.19e-20	0.224	407.5	5.84e-20	0.189	410.0	6.06e-20	0.154	412.5	6.49e-20	0.119	415.0	6.92e-20	0.084
417.5	6.87e-20	0.049	420.0	6.82e-20	0.014	422.5	6.71e-20	0.000	425.0	6.49e-20	0.000	427.5	5.95e-20	0.000
430.0	5.73e-20	0.000	432.5	6.28e-20	0.000	435.0	6.01e-20	0.000	437.5	5.84e-20	0.000	440.0	5.95e-20	0.000
442.5	6.49e-20	0.000	445.0	5.95e-20	0.000	447.5	4.98e-20	0.000	450.0	3.79e-20	0.000	452.5	2.81e-20	0.000
455.0	1.73e-20	0.000	457.5	1.08e-20	0.000	460.0	5.41e-21	0.000	462.5	3.79e-21	0.000	465.0	2.16e-21	0.000
467.5	1.08e-21	0.000	470.0	1.08e-21	0.000	472.5	0.00e+00	0.000						
BZCHO														
299.0	1.78e-19	1.000	304.0	7.40e-20	1.000	306.0	6.91e-20	1.000	309.0	6.41e-20	1.000	313.0	6.91e-20	1.000
314.0	6.91e-20	1.000	318.0	6.41e-20	1.000	325.0	8.39e-20	1.000	332.0	7.65e-20	1.000	338.0	8.88e-20	1.000
342.0	8.88e-20	1.000	346.0	7.89e-20	1.000	349.0	7.89e-20	1.000	354.0	9.13e-20	1.000	355.0	8.14e-20	1.000
364.0	5.67e-20	1.000	368.0	6.66e-20	1.000	369.0	8.39e-20	1.000	370.0	8.39e-20	1.000	372.0	3.45e-20	1.000
374.0	3.21e-20	1.000	376.0	2.47e-20	1.000	377.0	2.47e-20	1.000	380.0	3.58e-20	1.000	382.0	9.90e-21	1.000
386.0	0.00e+00	1.000												
ACROLEIN														
250.0	1.80e-21	1.000	252.0	2.05e-21	1.000	253.0	2.20e-21	1.000	254.0	2.32e-21	1.000	255.0	2.45e-21	1.000
256.0	2.56e-21	1.000	257.0	2.65e-21	1.000	258.0	2.74e-21	1.000	259.0	2.83e-21	1.000	260.0	2.98e-21	1.000
261.0	3.24e-21	1.000	262.0	3.47e-21	1.000	263.0	3.58e-21	1.000	264.0	3.93e-21	1.000	265.0	4.67e-21	1.000
266.0	5.10e-21	1.000	267.0	5.38e-21	1.000	268.0	5.73e-21	1.000	269.0	6.13e-21	1.000	270.0	6.64e-21	1.000
271.0	7.20e-21	1.000	272.0	7.77e-21	1.000	273.0	8.37e-21	1.000	274.0	8.94e-21	1.000	275.0	9.55e-21	1.000
276.0	1.04e-20	1.000	277.0	1.12e-20	1.000	278.0	1.19e-20	1.000	279.0	1.27e-20	1.000	280.0	1.27e-20	1.000
281.0	1.26e-20	1.000	282.0	1.26e-20	1.000	283.0	1.28e-20	1.000	284.0	1.33e-20	1.000	285.0	1.38e-20	1.000
286.0	1.44e-20	1.000	287.0	1.50e-20	1.000	288.0	1.57e-20	1.000	289.0	1.63e-20	1.000	290.0	1.71e-20	1.000
291.0	1.78e-20	1.000	292.0	1.86e-20	1.000	293.0	1.95e-20	1.000	294.0	2.05e-20	1.000	295.0	2.15e-20	1.000
296.0	2.26e-20	1.000	297.0	2.37e-20	1.000	298.0	2.48e-20	1.000	299.0	2.60e-20	1.000	300.0	2.73e-20	1.000
301.0	2.85e-20	1.000	302.0	2.99e-20	1.000	303.0	3.13e-20	1.000	304.0	3.27e-20	1.000	305.0	3.39e-20	1.000
306.0	3.51e-20	1.000	307.0	3.63e-20	1.000	308.0	3.77e-20	1.000	309.0	3.91e-20	1.000	310.0	4.07e-20	1.000
311.0	4.25e-20	1.000	312.0	4.39e-20	1.000	313.0	4.44e-20	1.000	314.0	4.50e-20	1.000	315.0	4.59e-20	1.000
316.0	4.75e-20	1.000	317.0	4.90e-20	1.000	318.0	5.05e-20	1.000	319.0	5.19e-20	1.000	320.0	5.31e-20	1.000
321.0	5.43e-20	1.000	322.0	5.52e-20	1.000	323.0	5.60e-20	1.000	324.0	5.67e-20	1.000	325.0	5.67e-20	1.000
326.0	5.62e-20	1.000	327.0	5.63e-20	1.000	328.0	5.71e-20	1.000	329.0	5.76e-20	1.000	330.0	5.80e-20	1.000
331.0	5.95e-20	1.000	332.0	6.23e-20	1.000	333.0	6.39e-20	1.000	334.0	6.38e-20	1.000	335.0	6.24e-20	1.000
336.0	6.01e-20	1.000	337.0	5.79e-20	1.000	338.0	5.63e-20	1.000	339.0	5.56e-20	1.000	340.0	5.52e-20	1.000
341.0	5.54e-20	1.000	342.0	5.53e-20	1.000	343.0	5.47e-20	1.000	344.0	5.41e-20	1.000	345.0	5.40e-20	1.000
346.0	5.48e-20	1.000	347.0	5.90e-20	1.000	348.0	6.08e-20	1.000	349.0	6.00e-20	1.000	350.0	5.53e-20	1.000
351.0	5.03e-20	1.000	352.0	4.50e-20	1.000	353.0	4.03e-20	1.000	354.0	3.75e-20	1.000	355.0	3.55e-20	1.000
356.0	3.45e-20	1.000	357.0	3.46e-20	1.000	358.0	3.49e-20	1.000	359.0	3.41e-20	1.000	360.0	3.23e-20	1.000
361.0	2.95e-20	1.000	362.0	2.81e-20	1.000	363.0	2.91e-20	1.000	364.0	3.25e-20	1.000	365.0	3.54e-20	1.000
366.0	3.30e-20	1.000	367.0	2.78e-20	1.000	368.0	2.15e-20	1.000	369.0	1.59e-20	1.000	370.0	1.19e-20	1.000
371.0	8.99e-21	1.000	372.0	7.22e-21	1.000	373.0	5.86e-21	1.000	374.0	4.69e-21	1.000	375.0	3.72e-21	1.000
376.0	3.57e-21	1.000	377.0	3.55e-21	1.000	378.0	2.83e-21	1.000	379.0	1.69e-21	1.000	380.0	8.29e-24	1.000
381.0	0.00e+00	1.000												
IC3ONO2														
185.0	1.79e-17	1.000	188.0	1.81e-17	1.000	190.0	1.79e-17	1.000	195.0	1.61e-17	1.000	200.0	1.26e-17	1.000
205.0	8.67e-18	1.000	210.0	4.98e-18	1.000	215.0	2.47e-18	1.000	220.0	1.17e-18	1.000	225.0	5.80e-19	1.000
230.0	3.10e-19	1.000	235.0	1.80e-19	1.000	240.0	1.10e-19	1.000	245.0	7.00e-20	1.000	250.0	5.70e-20	1.000

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
255.0	5.20e-20	1.000	260.0	4.90e-20	1.000	265.0	4.60e-20	1.000	270.0	4.10e-20	1.000	275.0	3.60e-20	1.000
280.0	2.90e-20	1.000	285.0	2.30e-20	1.000	290.0	1.70e-20	1.000	295.0	1.20e-20	1.000	300.0	8.10e-21	1.000
305.0	5.20e-21	1.000	310.0	3.20e-21	1.000	315.0	1.90e-21	1.000	320.0	1.10e-21	1.000	325.0	6.10e-22	1.000
330.0	3.70e-22	1.000	335.0	0.00e+00	1.000									
MGLY_ABS														
219.0	9.84e-21	1.000	219.5	1.04e-20	1.000	220.0	1.06e-20	1.000	220.5	1.11e-20	1.000	221.0	1.15e-20	1.000
221.5	1.18e-20	1.000	222.0	1.22e-20	1.000	222.5	1.24e-20	1.000	223.0	1.26e-20	1.000	223.5	1.26e-20	1.000
224.0	1.25e-20	1.000	224.5	1.24e-20	1.000	225.0	1.25e-20	1.000	225.5	1.27e-20	1.000	226.0	1.27e-20	1.000
226.5	1.29e-20	1.000	227.0	1.31e-20	1.000	227.5	1.32e-20	1.000	228.0	1.35e-20	1.000	228.5	1.37e-20	1.000
229.0	1.40e-20	1.000	229.5	1.42e-20	1.000	230.0	1.48e-20	1.000	230.5	1.53e-20	1.000	231.0	1.57e-20	1.000
231.5	1.59e-20	1.000	232.0	1.61e-20	1.000	232.5	1.62e-20	1.000	233.0	1.61e-20	1.000	233.5	1.68e-20	1.000
234.0	1.74e-20	1.000	234.5	1.80e-20	1.000	235.0	1.84e-20	1.000	235.5	1.87e-20	1.000	236.0	1.89e-20	1.000
236.5	1.91e-20	1.000	237.0	1.93e-20	1.000	237.5	1.94e-20	1.000	238.0	1.96e-20	1.000	238.5	1.96e-20	1.000
239.0	2.01e-20	1.000	239.5	2.04e-20	1.000	240.0	2.08e-20	1.000	240.5	2.10e-20	1.000	241.0	2.14e-20	1.000
241.5	2.16e-20	1.000	242.0	2.19e-20	1.000	242.5	2.20e-20	1.000	243.0	2.23e-20	1.000	243.5	2.26e-20	1.000
244.0	2.28e-20	1.000	244.5	2.29e-20	1.000	245.0	2.30e-20	1.000	245.5	2.32e-20	1.000	246.0	2.33e-20	1.000
246.5	2.35e-20	1.000	247.0	2.38e-20	1.000	247.5	2.41e-20	1.000	248.0	2.46e-20	1.000	248.5	2.51e-20	1.000
249.0	2.57e-20	1.000	249.5	2.61e-20	1.000	250.0	2.65e-20	1.000	250.5	2.67e-20	1.000	251.0	2.69e-20	1.000
251.5	2.69e-20	1.000	252.0	2.71e-20	1.000	252.5	2.72e-20	1.000	253.0	2.73e-20	1.000	253.5	2.74e-20	1.000
254.0	2.76e-20	1.000	254.5	2.78e-20	1.000	255.0	2.82e-20	1.000	255.5	2.87e-20	1.000	256.0	2.93e-20	1.000
256.5	2.98e-20	1.000	257.0	3.07e-20	1.000	257.5	3.12e-20	1.000	258.0	3.17e-20	1.000	258.5	3.21e-20	1.000
259.0	3.26e-20	1.000	259.5	3.28e-20	1.000	260.0	3.29e-20	1.000	260.5	3.31e-20	1.000	261.0	3.33e-20	1.000
261.5	3.34e-20	1.000	262.0	3.36e-20	1.000	262.5	3.38e-20	1.000	263.0	3.42e-20	1.000	263.5	3.44e-20	1.000
264.0	3.48e-20	1.000	264.5	3.54e-20	1.000	265.0	3.59e-20	1.000	265.5	3.65e-20	1.000	266.0	3.73e-20	1.000
266.5	3.80e-20	1.000	267.0	3.87e-20	1.000	267.5	3.95e-20	1.000	268.0	4.02e-20	1.000	268.5	4.08e-20	1.000
269.0	4.13e-20	1.000	269.5	4.17e-20	1.000	270.0	4.20e-20	1.000	270.5	4.22e-20	1.000	271.0	4.22e-20	1.000
271.5	4.22e-20	1.000	272.0	4.23e-20	1.000	272.5	4.24e-20	1.000	273.0	4.27e-20	1.000	273.5	4.29e-20	1.000
274.0	4.31e-20	1.000	274.5	4.33e-20	1.000	275.0	4.37e-20	1.000	275.5	4.42e-20	1.000	276.0	4.48e-20	1.000
276.5	4.56e-20	1.000	277.0	4.64e-20	1.000	277.5	4.71e-20	1.000	278.0	4.78e-20	1.000	278.5	4.83e-20	1.000
279.0	4.87e-20	1.000	279.5	4.90e-20	1.000	280.0	4.92e-20	1.000	280.5	4.93e-20	1.000	281.0	4.94e-20	1.000
281.5	4.92e-20	1.000	282.0	4.90e-20	1.000	282.5	4.86e-20	1.000	283.0	4.83e-20	1.000	283.5	4.79e-20	1.000
284.0	4.76e-20	1.000	284.5	4.72e-20	1.000	285.0	4.70e-20	1.000	285.5	4.68e-20	1.000	286.0	4.66e-20	1.000
286.5	4.65e-20	1.000	287.0	4.65e-20	1.000	287.5	4.68e-20	1.000	288.0	4.73e-20	1.000	288.5	4.78e-20	1.000
289.0	4.84e-20	1.000	289.5	4.89e-20	1.000	290.0	4.92e-20	1.000	290.5	4.92e-20	1.000	291.0	4.90e-20	1.000
291.5	4.86e-20	1.000	292.0	4.81e-20	1.000	292.5	4.75e-20	1.000	293.0	4.70e-20	1.000	293.5	4.65e-20	1.000
294.0	4.58e-20	1.000	294.5	4.48e-20	1.000	295.0	4.38e-20	1.000	295.5	4.27e-20	1.000	296.0	4.17e-20	1.000
296.5	4.07e-20	1.000	297.0	3.99e-20	1.000	297.5	3.94e-20	1.000	298.0	3.88e-20	1.000	298.5	3.82e-20	1.000
299.0	3.76e-20	1.000	299.5	3.72e-20	1.000	300.0	3.69e-20	1.000	300.5	3.68e-20	1.000	301.0	3.70e-20	1.000
301.5	3.72e-20	1.000	302.0	3.74e-20	1.000	302.5	3.74e-20	1.000	303.0	3.75e-20	1.000	303.5	3.71e-20	1.000
304.0	3.62e-20	1.000	304.5	3.51e-20	1.000	305.0	3.38e-20	1.000	305.5	3.25e-20	1.000	306.0	3.15e-20	1.000
306.5	3.04e-20	1.000	307.0	2.92e-20	1.000	307.5	2.80e-20	1.000	308.0	2.71e-20	1.000	308.5	2.63e-20	1.000
309.0	2.52e-20	1.000	309.5	2.43e-20	1.000	310.0	2.34e-20	1.000	310.5	2.25e-20	1.000	311.0	2.19e-20	1.000
311.5	2.12e-20	1.000	312.0	2.06e-20	1.000	312.5	2.02e-20	1.000	313.0	1.96e-20	1.000	313.5	1.92e-20	1.000
314.0	1.91e-20	1.000	314.5	1.88e-20	1.000	315.0	1.86e-20	1.000	315.5	1.85e-20	1.000	316.0	1.86e-20	1.000
316.5	1.87e-20	1.000	317.0	1.87e-20	1.000	317.5	1.87e-20	1.000	318.0	1.83e-20	1.000	318.5	1.75e-20	1.000
319.0	1.69e-20	1.000	319.5	1.60e-20	1.000	320.0	1.50e-20	1.000	320.5	1.41e-20	1.000	321.0	1.34e-20	1.000
321.5	1.27e-20	1.000	322.0	1.21e-20	1.000	322.5	1.18e-20	1.000	323.0	1.14e-20	1.000	323.5	1.08e-20	1.000
324.0	1.01e-20	1.000	324.5	9.62e-21	1.000	325.0	9.28e-21	1.000	325.5	8.75e-21	1.000	326.0	8.49e-21	1.000
326.5	8.21e-21	1.000	327.0	7.71e-21	1.000	327.5	7.38e-21	1.000	328.0	7.18e-21	1.000	328.5	6.86e-21	1.000
329.0	6.71e-21	1.000	329.5	6.63e-21	1.000	330.0	6.46e-21	1.000	330.5	6.29e-21	1.000	331.0	6.21e-21	1.000
331.5	6.18e-21	1.000	332.0	6.20e-21	1.000	332.5	5.49e-21	1.000	333.0	5.21e-21	1.000	333.5	5.38e-21	1.000
334.0	5.35e-21	1.000	334.5	5.04e-21	1.000	335.0	4.94e-21	1.000	335.5	4.90e-21	1.000	336.0	4.52e-21	1.000
336.5	4.26e-21	1.000	337.0	4.11e-21	1.000	337.5	3.76e-21	1.000	338.0	3.61e-21	1.000	338.5	3.58e-21	1.000
339.0	3.47e-21	1.000	339.5	3.32e-21	1.000	340.0	3.22e-21	1.000	340.5	3.10e-21	1.000	341.0	3.00e-21	1.000
341.5	2.94e-21	1.000	342.0	2.89e-21	1.000	342.5	2.86e-21	1.000	343.0	2.88e-21	1.000	343.5	2.88e-21	1.000
344.0	2.89e-21	1.000	344.5	2.91e-21	1.000	345.0	2.95e-21	1.000	345.5	3.00e-21	1.000	346.0	3.08e-21	1.000
346.5	3.18e-21	1.000	347.0	3.25e-21	1.000	347.5	3.30e-21	1.000	348.0	3.39e-21	1.000	348.5	3.51e-21	1.000
349.0	3.63e-21	1.000	349.5	3.73e-21	1.000	350.0	3.85e-21	1.000	350.5	3.99e-21	1.000	351.0	4.27e-21	1.000
351.5	4.47e-21	1.000	352.0	4.63e-21	1.000	352.5	4.78e-21	1.000	353.0	4.92e-21	1.000	353.5	5.07e-21	1.000
354.0	5.23e-21	1.000	354.5	5.39e-21	1.000	355.0	5.56e-21	1.000	355.5	5.77e-21	1.000	356.0	5.97e-21	1.000
356.5	6.15e-21	1.000	357.0	6.35e-21	1.000	357.5	6.56e-21	1.000	358.0	6.76e-21	1.000	358.5	6.95e-21	1.000
359.0	7.20e-21	1.000	359.5	7.44e-21	1.000	360.0	7.64e-21	1.000	360.5	7.89e-21	1.000	361.0	8.15e-21	1.000
361.5	8.43e-21	1.000	362.0	8.71e-21	1.000	362.5	9.02e-21	1.000	363.0	9.33e-21	1.000	363.5	9.65e-21	1.000
364.0	1.00e-20	1.000	364.5	1.04e-20	1.000	365.0	1.08e-20	1.000	365.5	1.11e-20	1.000	366.0	1.15e-20	1.000
366.5	1.19e-20	1.000	367.0	1.23e-20	1.000	367.5	1.27e-20	1.000	368.0	1.31e-20	1.000	368.5	1.35e-20	1.000
369.0	1.40e-20	1.000	369.5	1.44e-20	1.000	370.0	1.47e-20	1.000	370.5	1.51e-20	1.000	371.0	1.55e-20	1.000
371.5	1.59e-20	1.000	372.0	1.64e-20	1.000	372.5	1.70e-20	1.000	373.0	1.73e-20	1.000	373.5	1.77e-20	1.000
374.0	1.81e-20	1.000	374.5	1.86e-20	1.000	375.0	1.90e-20	1.000	375.5	1.96e-20	1.000	376.0	2.02e-20	1.000
376.5	2.06e-20	1.000	377.0	2.10e-20	1.000	377.5	2.14e-20	1.000	378.0	2.18e-20	1.000	378.5	2.24e-20	1.000
379.0	2.30e-20	1.000	379.5	2.37e-20	1.000	380.0	2.42e-20	1.000	380.5	2.47e-20	1.000	381.0	2.54e-20	1.000
381.5	2.62e-20	1.000	382.0	2.69e-20	1.000	382.5	2.79e-20	1.000	383.0	2.88e-20	1.000	383.5	2.96e-20	1.000
384.0	3.02e-20	1.000	384.5	3.10e-20	1.000	385.0	3.20e-20	1.000	385.5	3.29e-20	1.000	386.0	3.39e-20	1.000
386.5	3.51e-20	1.000	387.0	3.62e-20	1.000	387.5	3.69e-20	1.000	388.0	3.70e-20	1.000	388.5	3.77e-20	1.000

Table A-5 (continued)

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
389.0	3.88e-20	1.000	389.5	3.97e-20	1.000	390.0	4.03e-20	1.000	390.5	4.12e-20	1.000	391.0	4.22e-20	1.000
391.5	4.29e-20	1.000	392.0	4.30e-20	1.000	392.5	4.38e-20	1.000	393.0	4.47e-20	1.000	393.5	4.55e-20	1.000
394.0	4.56e-20	1.000	394.5	4.59e-20	1.000	395.0	4.67e-20	1.000	395.5	4.80e-20	1.000	396.0	4.87e-20	1.000
396.5	4.96e-20	1.000	397.0	5.08e-20	1.000	397.5	5.19e-20	1.000	398.0	5.23e-20	1.000	398.5	5.39e-20	1.000
399.0	5.46e-20	1.000	399.5	5.54e-20	1.000	400.0	5.59e-20	1.000	400.5	5.77e-20	1.000	401.0	5.91e-20	1.000
401.5	5.99e-20	1.000	402.0	6.06e-20	1.000	402.5	6.20e-20	1.000	403.0	6.35e-20	1.000	403.5	6.52e-20	1.000
404.0	6.54e-20	1.000	404.5	6.64e-20	1.000	405.0	6.93e-20	1.000	405.5	7.15e-20	1.000	406.0	7.19e-20	1.000
406.5	7.32e-20	1.000	407.0	7.58e-20	1.000	407.5	7.88e-20	1.000	408.0	7.97e-20	1.000	408.5	7.91e-20	1.000
409.0	8.11e-20	1.000	409.5	8.41e-20	1.000	410.0	8.53e-20	1.000	410.5	8.59e-20	1.000	411.0	8.60e-20	1.000
411.5	8.80e-20	1.000	412.0	9.04e-20	1.000	412.5	9.45e-20	1.000	413.0	9.34e-20	1.000	413.5	9.37e-20	1.000
414.0	9.63e-20	1.000	414.5	9.71e-20	1.000	415.0	9.70e-20	1.000	415.5	9.65e-20	1.000	416.0	9.69e-20	1.000
416.5	9.89e-20	1.000	417.0	1.00e-19	1.000	417.5	1.02e-19	1.000	418.0	1.00e-19	1.000	418.5	1.02e-19	1.000
419.0	1.01e-19	1.000	419.5	1.01e-19	1.000	420.0	1.03e-19	1.000	420.5	1.01e-19	1.000	421.0	1.04e-19	1.000
421.5	1.05e-19	1.000	422.0	1.06e-19	1.000	422.5	1.04e-19	1.000	423.0	1.05e-19	1.000	423.5	1.05e-19	1.000
424.0	1.01e-19	1.000	424.5	1.01e-19	1.000	425.0	1.05e-19	1.000	425.5	1.03e-19	1.000	426.0	1.02e-19	1.000
426.5	1.01e-19	1.000	427.0	9.77e-20	1.000	427.5	9.81e-20	1.000	428.0	1.00e-19	1.000	428.5	1.02e-19	1.000
429.0	9.89e-20	1.000	429.5	9.85e-20	1.000	430.0	1.04e-19	1.000	430.5	1.08e-19	1.000	431.0	1.05e-19	1.000
431.5	1.02e-19	1.000	432.0	9.64e-20	1.000	432.5	1.01e-19	1.000	433.0	1.06e-19	1.000	433.5	1.09e-19	1.000
434.0	1.04e-19	1.000	434.5	1.03e-19	1.000	435.0	1.07e-19	1.000	435.5	1.16e-19	1.000	436.0	1.09e-19	1.000
436.5	1.11e-19	1.000	437.0	9.81e-20	1.000	437.5	9.71e-20	1.000	438.0	1.06e-19	1.000	438.5	1.16e-19	1.000
439.0	1.08e-19	1.000	439.5	1.05e-19	1.000	440.0	9.70e-20	1.000	440.5	1.01e-19	1.000	441.0	1.04e-19	1.000
441.5	1.07e-19	1.000	442.0	1.02e-19	1.000	442.5	9.68e-20	1.000	443.0	1.00e-19	1.000	443.5	1.14e-19	1.000
444.0	1.13e-19	1.000	444.5	1.03e-19	1.000	445.0	9.74e-20	1.000	445.5	8.46e-20	1.000	446.0	8.70e-20	1.000
446.5	9.97e-20	1.000	447.0	1.01e-19	1.000	447.5	9.15e-20	1.000	448.0	9.41e-20	1.000	448.5	8.99e-20	1.000
449.0	1.10e-19	1.000	449.5	9.12e-20	1.000	450.0	8.56e-20	1.000	450.5	8.28e-20	1.000	451.0	6.15e-20	1.000
451.5	5.56e-20	1.000	452.0	6.47e-20	1.000	452.5	7.27e-20	1.000	453.0	5.75e-20	1.000	453.5	5.08e-20	1.000
454.0	4.38e-20	1.000	454.5	3.81e-20	1.000	455.0	3.61e-20	1.000	455.5	3.61e-20	1.000	456.0	3.13e-20	1.000
456.5	2.72e-20	1.000	457.0	2.44e-20	1.000	457.5	2.22e-20	1.000	458.0	1.82e-20	1.000	458.5	1.43e-20	1.000
459.0	1.32e-20	1.000	459.5	1.05e-20	1.000	460.0	8.95e-21	1.000	460.5	8.90e-21	1.000	461.0	7.94e-21	1.000
461.5	7.04e-21	1.000	462.0	6.46e-21	1.000	462.5	5.63e-21	1.000	463.0	4.78e-21	1.000	463.5	3.94e-21	1.000
464.0	3.26e-21	1.000	464.5	2.97e-21	1.000	465.0	2.65e-21	1.000	465.5	2.46e-21	1.000	466.0	2.27e-21	1.000
466.5	2.08e-21	1.000	467.0	1.86e-21	1.000	467.5	1.76e-21	1.000	468.0	1.60e-21	1.000	468.5	1.44e-21	1.000
469.0	1.34e-21	1.000	469.5	1.20e-21	1.000	470.0	1.07e-21	1.000	470.5	1.02e-21	1.000	471.0	9.92e-22	1.000
471.5	9.97e-22	1.000	472.0	8.87e-22	1.000	472.5	8.27e-22	1.000	473.0	7.76e-22	1.000	473.5	7.15e-22	1.000
474.0	6.71e-22	1.000	474.5	6.67e-22	1.000	475.0	6.10e-22	1.000	475.5	6.17e-22	1.000	476.0	5.54e-22	1.000
476.5	5.22e-22	1.000	477.0	5.10e-22	1.000	477.5	5.17e-22	1.000	478.0	4.80e-22	1.000	478.5	4.71e-22	1.000
479.0	4.60e-22	1.000	479.5	4.35e-22	1.000	480.0	3.90e-22	1.000	480.5	3.71e-22	1.000	481.0	3.62e-22	1.000
481.5	3.52e-22	1.000	482.0	3.05e-22	1.000	482.5	3.05e-22	1.000	483.0	2.86e-22	1.000	483.5	2.53e-22	1.000
484.0	2.75e-22	1.000	484.5	2.59e-22	1.000	485.0	2.47e-22	1.000	485.5	2.36e-22	1.000	486.0	2.12e-22	1.000
486.5	1.89e-22	1.000	487.0	1.93e-22	1.000	487.5	1.86e-22	1.000	488.0	1.82e-22	1.000	488.5	1.75e-22	1.000
489.0	1.74e-22	1.000	489.5	1.72e-22	1.000	490.0	1.66e-22	1.000	490.5	1.75e-22	1.000	491.0	1.54e-22	1.000
491.5	1.74e-22	1.000	492.0	1.63e-22	1.000	492.5	1.53e-22	1.000	493.0	1.52e-22	1.000	493.5	5.85e-23	1.000
494.0	0.00e+00	1.000												

Table A-6. Listing of the reactions of the individual VOCs that can be represented explicitly, but are not part of the base mechanism.

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Methane	6.36e-15	2.15e-12	3.45	0.0	METHANE + HO. = C-O2.
Ethane	2.54e-13	1.37e-12	0.99	2.0	ETHANE + HO. = RO2-R. + CCHO
Propane	1.13e-12	1.40e-12	0.12	2.0	PROPANE + HO. = #.965 RO2-R. + #.035 RO2-N. + #.261 RCHO + #.704 ACET + #-0.104 XC
n-Butane [LP]	2.44e-12	1.52e-12	-0.29	2.0	N-C4 + HO. = #.921 RO2-R. + #.079 RO2-N. + #.413 R2O2. + #.632 CCHO + #.12 RCHO + #.485 MEK + #-0.038 XC
n-Butane [AP]	2.44e-12	1.52e-12	-0.29	2.0	N-C4 + HO. = #.921 RO2-R. + #.079 RO2-N. + #.413 R2O2. + #.632 CCHO + #.485 MEK + #-0.038 XC + #.12 PRD1
	2.52e-11	2.52e-11			PRD1 + HO. = #.122 HO2. + #.086 RO2-R. + #.004 RO2-N. + #.003 R2O2. + #.787 RCO-O2. + #.037 CO + #.045 HCHO + #.003 CCHO + #.206 RCHO + #-0.092 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.99 HO2. + #1.005 RO2-R. + #.004 RO2-N. + CO + #.026 HCHO + #.002 CCHO + #.986 RCHO + #-1.013 XC
n-Pentane [LP]	4.01e-12	2.20e-12	-0.36	2.0	N-C5 + HO. = #.855 RO2-R. + #.145 RO2-N. + #.65 R2O2. + #.147 CCHO + #.22 RCHO + #.238 MEK + #.397 PROD2 + #-0.157 XC
n-Pentane [AP]	4.01e-12	2.20e-12	-0.36	2.0	N-C5 + HO. = #.855 RO2-R. + #.145 RO2-N. + #.65 R2O2. + #.147 CCHO + #.147 RCHO + #.238 MEK + #-0.157 XC + #.073 PRD1 + #.397 PRD2
	3.01e-11	3.01e-11			PRD1 + HO. = #.276 HO2. + #.074 RO2-R. + #.005 RO2-N. + #.645 RCO-O2. + #.025 CO + #.045 CCHO + #.348 RCHO + #.001 MGLY + #-0.13 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.215 HO2. + #1.715 RO2-R. + #.07 RO2-N. + CO + #.93 RCHO + #-1.211 XC
	9.63e-12	9.63e-12			PRD2 + HO. = #.34 HO2. + #.529 RO2-R. + #.037 RO2-N. + #.084 CCO-O2. + #.01 RCO-O2. + #.444 HCHO + #.953 RCHO + #2.277 XC
		PF=KETONE QY = 5.0e-2			PRD2 + HV = RO2-R. + #.013 R2O2. + CCO-O2. + #.033 HCHO + #.002 CCHO + #.987 RCHO + XC
n-Hexane [LP]	5.47e-12	1.38e-12	-0.82	2.0	N-C6 + HO. = #.775 RO2-R. + #.225 RO2-N. + #.787 R2O2. + #.011 CCHO + #.113 RCHO + #.688 PROD2 + #.162 XC
n-Hexane [AP]	5.47e-12	1.38e-12	-0.82	2.0	N-C6 + HO. = #.775 RO2-R. + #.225 RO2-N. + #.787 R2O2. + #.011 CCHO + #.051 RCHO + #.162 XC + #.062 PRD1 + #.688 PRD2
	3.32e-11	3.32e-11			PRD1 + HO. = #.278 HO2. + #.124 RO2-R. + #.013 RO2-N. + #.585 RCO-O2. + #.009 CO + #.017 CCHO + #.427 RCHO + #.013 MGLY + #-0.199 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.077 CCHO + #.874 RCHO + #-1.531 XC
	1.19e-11	1.19e-11			PRD2 + HO. = #.362 HO2. + #.456 RO2-R. + #.055 RO2-N. + #.06 R2O2. + #.027 CCO-O2. + #.1 RCO-O2. + #.183 HCHO + #.192 CCHO + #.58 RCHO + #.031 MEK + #.28 PROD2 + #1.204 XC
		PF=KETONE QY = 2.3e-2			PRD2 + HV = #.965 RO2-R. + #.035 RO2-N. + #.372 R2O2. + #.467 CCO-O2. + #.533 RCO-O2. + #.015 HCHO + #.001 CCHO + #.96 RCHO + #.363 XC
n-Heptane [LP]	7.02e-12	1.43e-12	-0.95	2.0	N-C7 + HO. = #.705 RO2-R. + #.295 RO2-N. + #.799 R2O2. + #.055 RCHO + #.659 PROD2 + #1.11 XC
n-Heptane [AP]	7.02e-12	1.43e-12	-0.95	2.0	N-C7 + HO. = #.705 RO2-R. + #.295 RO2-N. + #.799 R2O2. + #.009 RCHO + #1.11 XC + #.046 PRD1 + #.659 PRD2
	3.46e-11	3.46e-11			PRD1 + HO. = #.235 HO2. + #.176 RO2-R. + #.028 RO2-N. + #.561 RCO-O2. + #.006 CO + #.479 RCHO + #.013 MGLY + #-0.331 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.898 RCHO + #-1.807 XC
	1.57e-11	1.57e-11			PRD2 + HO. = #.409 HO2. + #.431 RO2-R. + #.066 RO2-N. + #.016 CCO-O2. + #.078 RCO-O2. + #.066 HCHO + #.166 CCHO + #.499 RCHO + #.491 PROD2 + #.494 XC
		PF=KETONE QY = 1.0e-2			PRD2 + HV = #.919 RO2-R. + #.081 RO2-N. + #.688 R2O2. + #.362 CCO-O2. + #.638 RCO-O2. + #.028 CCHO + #.919 RCHO + #.064 XC
n-Octane [LP]	8.70e-12	2.48e-12	-0.75	2.0	N-C8 + HO. = #.646 RO2-R. + #.354 RO2-N. + #.786 R2O2. + #.024 RCHO + #.622 PROD2 + #2.073 XC
n-Octane [AP]	8.70e-12	2.48e-12	-0.75	2.0	N-C8 + HO. = #.646 RO2-R. + #.354 RO2-N. + #.786 R2O2. + #.024 RCHO + #2.073 XC + #.622 PRD1
	1.85e-11	1.85e-11			PRD1 + HO. = #.386 HO2. + #.431 RO2-R. + #.089 RO2-N. + #.019 CCO-O2. + #.075 RCO-O2. + #.013 HCHO + #.116 CCHO + #.48 RCHO + #.562 PROD2 + #.142 XC
n-Nonane [LP]	9.99e-12	2.26e-12	-0.89	2.0	N-C9 + HO. = #.602 RO2-R. + #.398 RO2-N. + #.777 R2O2. + #.018 RCHO + #.584 PROD2 + #3.055 XC
n-Nonane [AP]	9.99e-12	2.26e-12	-0.89	2.0	N-C9 + HO. = #.602 RO2-R. + #.398 RO2-N. + #.777 R2O2. + #.018 RCHO + #3.055 XC + #.584 PRD1
	2.05e-11	2.05e-11			PRD1 + HO. = #.335 HO2. + #.463 RO2-R. + #.116 RO2-N. + #.014 CCO-O2. + #.072 RCO-O2. + #.014 HCHO + #.072 CCHO + #.518 RCHO + #.544 PROD2 + #.083 XC
n-Decane [LP]	1.12e-11	2.82e-12	-0.83	2.0	N-C10 + HO. = #.572 RO2-R. + #.428 RO2-N. + #.772 R2O2. + #.015 RCHO + #.557 PROD2 + #4.045 XC
n-Decane [AP]	1.12e-11	2.82e-12	-0.83	2.0	N-C10 + HO. = #.572 RO2-R. + #.428 RO2-N. + #.772 R2O2. + #.015 RCHO + #4.045 XC + #.557 PRD1
	2.22e-11	2.22e-11			PRD1 + HO. = #.261 HO2. + #.509 RO2-R. + #.147 RO2-N. + #.009 CCO-O2. + #.074 RCO-O2. + #.012 HCHO + #.051 CCHO + #.497 RCHO + #.537 PROD2 + #.052 XC
n-Undecane [LP]	1.29e-11	1.29e-11			N-C11 + HO. = #.553 RO2-R. + #.447 RO2-N. + #.771 R2O2. + #.013 RCHO + #.54 PROD2 + #5.038 XC
n-Undecane [AP]	1.29e-11	1.29e-11			N-C11 + HO. = #.553 RO2-R. + #.447 RO2-N. + #.771 R2O2. + #.013 RCHO + #5.038 XC + #.54 PRD1
	2.38e-11	2.38e-11			PRD1 + HO. = #.201 HO2. + #.549 RO2-R. + #.174 RO2-N. + #.007 CCO-O2. + #.068 RCO-O2. + #.009 HCHO + #.041 CCHO + #.463 RCHO + #.536 PROD2 + #.04 XC
n-Dodecane [LP]	1.39e-11	1.39e-11			N-C12 + HO. = #.542 RO2-R. + #.458 RO2-N. + #.768 R2O2. + #.011 RCHO + #.53 PROD2 + #6.034 XC
n-Dodecane [AP]	1.39e-11	1.39e-11			N-C12 + HO. = #.542 RO2-R. + #.458 RO2-N. + #.768 R2O2. + #.011 RCHO + #6.034 XC + #.53 PRD1
	2.53e-11	2.53e-11			PRD1 + HO. = #.141 HO2. + #.588 RO2-R. + #.199 RO2-N. + #.004 R2O2. + #.006 CCO-O2. + #.066 RCO-O2. + #.007 HCHO + #.034 CCHO + #.425 RCHO + #.536 PROD2 + #.032 XC
n-Tridecane [LP]	1.60e-11	1.60e-11			N-C13 + HO. = #.535 RO2-R. + #.465 RO2-N. + #.766 R2O2. + #.01 RCHO + #.525 PROD2 + #7.03 XC
n-Tridecane [AP]	1.60e-11	1.60e-11			N-C13 + HO. = #.535 RO2-R. + #.465 RO2-N. + #.766 R2O2. + #.01 RCHO + #7.03 XC + #.525 PRD1
	2.69e-11	2.69e-11			PRD1 + HO. = #.094 HO2. + #.621 RO2-R. + #.218 RO2-N. + #.006 R2O2. + #.005 CCO-O2. + #.061 RCO-O2. + #.006 HCHO + #.029 CCHO + #.4 RCHO + #.534 PROD2 + #.027 XC
n-Tetradecane [LP]	1.80e-11	1.80e-11			N-C14 + HO. = #.53 RO2-R. + #.47 RO2-N. + #.765 R2O2. + #.009 RCHO + #.521 PROD2 + #8.027 XC
n-Tetradecane [AP]	1.80e-11	1.80e-11			N-C14 + HO. = #.53 RO2-R. + #.47 RO2-N. + #.765 R2O2. + #.009 RCHO + #8.027 XC + #.521 PRD1

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.84e-11	2.84e-11			PRD1 + HO. = #.051 HO2. + #.652 RO2-R. + #.235 RO2-N. + #.008 R2O2. + #.004 CCO-O2. + #.058 RCO-O2. + #.005 HCHO + #.025 CCHO + #.375 RCHO + #.534 PROD2 + #.023 XC
n-Pentadecane [LP]	2.10e-11	2.10e-11			N-C15 + HO. = #.527 RO2-R. + #.473 RO2-N. + #.764 R2O2. + #.008 RCHO + #.519 PROD2 + #9.025 XC
n-Pentadecane [AP]	2.10e-11	2.10e-11			N-C15 + HO. = #.527 RO2-R. + #.473 RO2-N. + #.764 R2O2. + #.008 RCHO + #9.025 XC + #.519 PRD1
	2.99e-11	2.99e-11			PRD1 + HO. = #.019 HO2. + #.674 RO2-R. + #.249 RO2-N. + #.015 R2O2. + #.004 CCO-O2. + #.055 RCO-O2. + #.004 HCHO + #.022 CCHO + #.357 RCHO + #.533 PROD2 + #.02 XC
n-C16 [LP]	2.30e-11	2.30e-11			N-C16 + HO. = #.525 RO2-R. + #.475 RO2-N. + #.763 R2O2. + #.008 RCHO + #.517 PROD2 + #10.023 XC
n-C16 [AP]	2.30e-11	2.30e-11			N-C16 + HO. = #.525 RO2-R. + #.475 RO2-N. + #.763 R2O2. + #.008 RCHO + #10.023 XC + #.517 PRD1
	3.14e-11	3.14e-11			PRD1 + HO. = #.002 HO2. + #.681 RO2-R. + #.261 RO2-N. + #.035 R2O2. + #.003 CCO-O2. + #.052 RCO-O2. + #.004 HCHO + #.019 CCHO + #.338 RCHO + #.533 PROD2 + #.018 XC
Isobutane [LP]	2.18e-12	1.04e-12	-0.45	2.0	2-ME-C3 + HO. = #.198 RO2-R. + #.042 RO2-N. + #.833 R2O2. + #.76 TBU-O. + #.073 HCHO + #.128 RCHO + #.07 ACET + #.8 XC
Isobutane [AP]	2.18e-12	1.04e-12	-0.45	2.0	2-ME-C3 + HO. = #.198 RO2-R. + #.042 RO2-N. + #.833 R2O2. + #.76 TBU-O. + #.073 HCHO + #.07 ACET + #.8 XC + #.128 PRD1
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
Isopentane [LP]	3.70e-12	3.70e-12			2-ME-C4 + HO. = #.881 RO2-R. + #.095 RO2-N. + #.902 R2O2. + #.024 C-O2. + #.012 HCHO + #.78 CCHO + #.101 RCHO + #.762 ACET + #.038 MEK + #.094 XC
Iso-Pentane [AP]	3.70e-12	3.70e-12			2-ME-C4 + HO. = #.881 RO2-R. + #.095 RO2-N. + #.902 R2O2. + #.024 C-O2. + #.012 HCHO + #.78 CCHO + #.762 ACET + #.038 MEK + #.094 XC + #.101 PRD1
	2.70e-11	2.70e-11			PRD1 + HO. = #.147 HO2. + #.124 RO2-R. + #.009 RO2-N. + #.721 RCO-O2. + #.053 CO + #.067 HCHO + #.006 CCHO + #.229 RCHO + #.039 PROD2 + #-0.266 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.465 HO2. + #1.491 RO2-R. + #.044 RO2-N. + CO + #.969 HCHO + #.578 CCHO + #.082 RCHO + #.344 PROD2 + #-2.697 XC
Neopentane	8.47e-13	1.62e-12	0.38	2.0	22-DM-C3 + HO. = #.021 RO2-R. + #.088 RO2-N. + #1.819 R2O2. + #.891 TBU-O. + #.928 HCHO + #.021 RCHO + #.809 XC
2,2-Dimethyl Butane [LP]	2.34e-12	3.22e-11	1.55		22-DM-C4 + HO. = #.304 RO2-R. + #.176 RO2-N. + #1.581 R2O2. + #.009 C-O2. + #.51 TBU-O. + #.227 HCHO + #.73 CCHO + #.103 RCHO + #.202 ACET + #.009 MEK + #.765 XC
2,2-Dimethyl Butane [AP]	2.34e-12	3.22e-11	1.55		22-DM-C4 + HO. = #.304 RO2-R. + #.176 RO2-N. + #1.581 R2O2. + #.009 C-O2. + #.51 TBU-O. + #.227 HCHO + #.73 CCHO + #.202 ACET + #.009 MEK + #.765 XC + #.103 PRD1
	2.48e-11	2.48e-11			PRD1 + HO. = #.136 HO2. + #.073 RO2-R. + #.007 RO2-N. + #.784 RCO-O2. + #.023 CO + #.027 HCHO + #.009 CCHO + #.192 RCHO + #.017 ACET + #.009 GLY + #-0.108 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + #-0 XC + XN PRD1 + HV = #.065 HO2. + #1.802 RO2-R. + #.133 RO2-N. + CO + #1.703 HCHO + #.05 CCHO + #.867 ACET + #-3.201 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
2,3-Dimethyl Butane [LP]	5.80e-12	1.12e-12	-0.98	2.0	23-DM-C4 + HO. = #.858 RO2-R. + #.142 RO2-N. + #.918 R2O2. + #.028 HCHO + #.023 CCHO + #.078 RCHO + #1.569 ACET + #.001 MEK + #.132 XC
2,3-Dimethyl Butane [AP]	5.80e-12	1.12e-12	-0.98	2.0	23-DM-C4 + HO. = #.858 RO2-R. + #.142 RO2-N. + #.918 R2O2. + #.028 HCHO + #.023 CCHO + #1.569 ACET + #.001 MEK + #.132 XC + #.078 PRD1
	2.85e-11	2.85e-11			PRD1 + HO. = #.132 HO2. + #.164 RO2-R. + #.017 RO2-N. + #.688 RCO-O2. + #.065 CO + #.087 HCHO + #.011 CCHO + #.228 RCHO + #.01 MEK + #.056 PROD2 + #.002 MGLY + #-0.404 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.065 HO2. + #1.856 RO2-R. + #.079 RO2-N. + CO + #.921 HCHO + #1.856 CCHO + #-3.107 XC
2-Methyl Pentane [LP]	5.30e-12	5.30e-12			2-ME-C5 + HO. = #.816 RO2-R. + #.184 RO2-N. + #.859 R2O2. + #.004 HCHO + #.011 CCHO + #.661 RCHO + #.346 ACET + #.006 MEK + #.153 PROD2 + #.904 XC
2-Methyl Pentane [AP]	5.30e-12	5.30e-12			2-ME-C5 + HO. = #.816 RO2-R. + #.184 RO2-N. + #.859 R2O2. + #.004 HCHO + #.011 CCHO + #.348 RCHO + #.346 ACET + #.006 MEK + #.904 XC + #.313 PRD1 + #.153 PRD2
	2.36e-11	2.36e-11			PRD1 + HO. = #.045 HO2. + #.106 RO2-R. + #.012 RO2-N. + #.005 R2O2. + #.838 RCO-O2. + #.035 CO + #.012 HCHO + #.007 CCHO + #.14 RCHO + #.049 ACET + #.009 PROD2 + #.002 MGLY + #-0.27 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + #-0 XC + XN PRD1 + HV = #.164 HO2. + #1.718 RO2-R. + #.118 RO2-N. + CO + #.369 HCHO + #.047 CCHO + #.421 RCHO + #.438 PROD2 + #-3.061 XC
	1.45e-11	1.45e-11			PRD2 + HO. = #.201 HO2. + #.666 RO2-R. + #.071 RO2-N. + #.062 CCO-O2. + #.612 HCHO + #.007 CCHO + #.345 RCHO + #.577 MEK + #1.483 XC
	PF=KETONE QY = 2.0e-2				PRD2 + HV = #.949 RO2-R. + #.051 RO2-N. + #.748 R2O2. + CCO-O2. + #1.484 HCHO + #.736 CCHO + #.213 RCHO + #.1 XC
3-Methylpentane [LP]	5.40e-12	5.40e-12			3-ME-C5 + HO. = #.844 RO2-R. + #.156 RO2-N. + #.989 R2O2. + #.005 HCHO + #.986 CCHO + #.069 RCHO + #.629 MEK + #.036 PROD2 + #.151 XC
3-Methylpentane [AP]	5.40e-12	5.40e-12			3-ME-C5 + HO. = #.844 RO2-R. + #.156 RO2-N. + #.989 R2O2. + #.005 HCHO + #.986 CCHO + #.001 RCHO + #.629 MEK + #.151 XC + #.036 PRD1 + #.068 PRD2
	1.11e-11	1.11e-11			PRD1 + HO. = #.145 HO2. + #.609 RO2-R. + #.063 RO2-N. + #.183 CCO-O2. + #.329 HCHO + #.074 CCHO + #.753 RCHO + #.147 PROD2 + #1.633 XC
	PF=KETONE QY = 2.0e-2				PRD1 + HV = #.961 RO2-R. + #.039 RO2-N. + #.4 R2O2. + CCO-O2. + #.645 HCHO + #.478 CCHO + #.56 PROD2 + #-1.199 XC
	3.18e-11	3.18e-11			PRD2 + HO. = #.262 HO2. + #.112 RO2-R. + #.012 RO2-N. + #.614 RCO-O2. + #.022 CO + #.001 HCHO + #.085 CCHO + #.372 RCHO + #.001 MGLY + #-0.23 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.143 HO2. + #1.75 RO2-R. + #.107 RO2-N. + CO + #.451 HCHO + #.871 CCHO + #.457 RCHO + #-2.208 XC
2,2,3-Trimethyl Butane [LP]	4.24e-12	7.61e-13	-1.03	2.0	223TM-C4 + HO. = #.183 RO2-R. + #.192 RO2-N. + #1.631 R2O2. + #.625 TBU-O. + #.16 HCHO + #.022 CCHO + #.065 RCHO + #.87 ACET + #.964 XC
2,2,3-Trimethyl Butane [AP]	4.24e-12	7.61e-13	-1.03	2.0	223TM-C4 + HO. = #.183 RO2-R. + #.192 RO2-N. + #1.631 R2O2. + #.625 TBU-O. + #.16 HCHO + #.022 CCHO + #.87 ACET + #.964 XC + #.065 PRD1

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.57e-11	2.57e-11			PRD1 + HO. = #.103 HO2. + #.12 RO2-R. + #.017 RO2-N. + #.761 RCO-O2. + #.019 CO + #.054 HCHO + #.001 CCHO + #.165 RCHO + #.038 ACET + #.001 MEK + #.019 PROD2 + #.043 MGLY + #-0.309 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #1.715 RO2-R. + #.188 RO2-N. + CO + #.812 HCHO + #.902 CCHO + #.812 ACET + #-4.18 XC
2,2-Dimethyl Pentane [LP]	3.40e-12	3.40e-12			22-DM-C5 + HO. = #.441 RO2-R. + #.209 RO2-N. + #1.191 R2O2. + #.35 TBU-O. + #.056 HCHO + #.017 CCHO + #.516 RCHO + #.014 ACET + #.017 MEK + #.257 PROD2 + #1.408 XC
2,2-Dimethyl Pentane [AP]	3.40e-12	3.40e-12			22-DM-C5 + HO. = #.441 RO2-R. + #.209 RO2-N. + #1.191 R2O2. + #.35 TBU-O. + #.056 HCHO + #.017 CCHO + #.363 RCHO + #.014 ACET + #.017 MEK + #1.408 XC + #.153 PRD1 + #.257 PRD2
	2.70e-11	2.70e-11			PRD1 + HO. = #.175 HO2. + #.06 RO2-R. + #.015 RO2-N. + #.046 R2O2. + #.732 RCO-O2. + #.017 TBU-O. + #.02 CO + #.003 HCHO + #.016 CCHO + #.252 RCHO + #.011 ACET + #.002 MGLY + #-0.191 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.096 HO2. + #1.75 RO2-R. + #.154 RO2-N. + CO + #.599 HCHO + #.379 CCHO + #.458 RCHO + #.395 ACET + #-2.838 XC
	5.50e-12	5.50e-12			PRD2 + HO. = #.465 HO2. + #.313 RO2-R. + #.041 RO2-N. + #.165 CCO-O2. + #.016 RCO-O2. + #.179 HCHO + #.866 RCHO + #.029 ACET + #.048 MEK + #2.32 XC
		PF=KETONE QY = 1.0e-2			PRD2 + HV = #.842 RO2-R. + #.158 RO2-N. + #.935 R2O2. + CCO-O2. + #1.777 HCHO + #.842 ACET + #-1.252 XC
2,3-Dimethyl Pentane [LP]	7.15e-12	7.15e-12			23-DM-C5 + HO. = #.783 RO2-R. + #.217 RO2-N. + #1.09 R2O2. + #.015 HCHO + #.453 CCHO + #.061 RCHO + #.733 ACET + #.517 MEK + #.01 PROD2 + #.269 XC
2,3-Dimethyl Pentane [AP]	7.15e-12	7.15e-12			23-DM-C5 + HO. = #.783 RO2-R. + #.217 RO2-N. + #1.09 R2O2. + #.015 HCHO + #.453 CCHO + #.003 RCHO + #.733 ACET + #.517 MEK + #.01 PROD2 + #.269 XC + #.058 PRD1
	3.29e-11	3.29e-11			PRD1 + HO. = #.254 HO2. + #.129 RO2-R. + #.02 RO2-N. + #.597 RCO-O2. + #.045 CO + #.084 CCHO + #.336 RCHO + #.045 PROD2 + #.003 MGLY + #-0.409 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #1.772 RO2-R. + #.13 RO2-N. + CO + #.006 HCHO + #2.593 CCHO + #.006 RCHO + #.01 PROD2 + #-4.05 XC
2,4-Dimethyl Pentane [LP]	5.00e-12	5.00e-12			24-DM-C5 + HO. = #.796 RO2-R. + #.204 RO2-N. + #1.323 R2O2. + #.333 HCHO + #.016 CCHO + #.562 RCHO + #.483 ACET + #.013 MEK + #.135 PROD2 + #1.413 XC
2,4-Dimethyl Pentane [AP]	5.00e-12	5.00e-12			24-DM-C5 + HO. = #.796 RO2-R. + #.204 RO2-N. + #1.323 R2O2. + #.333 HCHO + #.016 CCHO + #.483 ACET + #.013 MEK + #1.413 XC + #.562 PRD1 + #.135 PRD2
	2.47e-11	2.47e-11			PRD1 + HO. = #.106 RO2-R. + #.012 RO2-N. + #.007 R2O2. + #.882 RCO-O2. + #.074 CO + #.011 HCHO + #.006 CCHO + #.032 RCHO + #.061 ACET + #.031 MEK + #-0.22 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.622 HO2. + #1.276 RO2-R. + #.102 RO2-N. + CO + #.138 HCHO + #.037 CCHO + #.559 ACET + #.031 MEK + #.308 PROD2 + #-2.473 XC
	1.29e-11	1.29e-11			PRD2 + HO. = #.735 HO2. + #.135 RO2-R. + #.014 RO2-N. + #.105 CCO-O2. + #.011 RCO-O2. + #.072 HCHO + #.588 RCHO + #.387 MEK + #2.29 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=KETONE QY = 2.4e-2				PRD2 + HV = #.968 RO2-R. + #.032 RO2-N. + CCO-O2. + #.968 HCHO + #.331 CCHO + #.637 MEK + #-0.371 XC
2-Methyl Hexane [LP]	6.89e-12	6.89e-12			2-ME-C6 + HO. = #.731 RO2-R. + #.269 RO2-N. + #.906 R2O2. + #.022 HCHO + #.048 CCHO + #.236 RCHO + #.137 ACET + #.508 PROD2 + #1.102 XC
2-Methyl Hexane [AP]	6.89e-12	6.89e-12			2-ME-C6 + HO. = #.731 RO2-R. + #.269 RO2-N. + #.906 R2O2. + #.022 HCHO + #.048 CCHO + #.011 RCHO + #.137 ACET + #1.102 XC + #.224 PRD1 + #.508 PRD2
	2.56e-11	2.56e-11			PRD1 + HO. = #.062 HO2. + #.095 RO2-R. + #.01 RO2-N. + #.012 R2O2. + #.832 RCO-O2. + #.051 CO + #.011 HCHO + #.02 CCHO + #.143 RCHO + #.009 PROD2 + #-0.145 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.805 HO2. + #1.139 RO2-R. + #.056 RO2-N. + CO + #.157 CCHO + #.925 RCHO + #.019 PROD2 + #-1.539 XC
	8.59e-12	8.59e-12			PRD2 + HO. = #.041 HO2. + #.704 RO2-R. + #.124 RO2-N. + #.11 R2O2. + #.095 CCO-O2. + #.036 RCO-O2. + #.189 HCHO + #.011 CCHO + #.681 RCHO + #.495 ACET + #.139 MEK + #.033 PROD2 + #.463 XC
	PF=KETONE QY = 1.0e-2				PRD2 + HV = #.899 RO2-R. + #.101 RO2-N. + #.816 R2O2. + #.73 CCO-O2. + #.27 RCO-O2. + #.689 HCHO + #.199 CCHO + #.412 RCHO + #.288 PROD2 + #-0.928 XC
3,3-Dimethyl Pentane	3.00e-12	3.00e-12			33-DM-C5 + HO. = #.737 RO2-R. + #.238 RO2-N. + #1.593 R2O2. + #.025 C-O2. + #.163 HCHO + #1.328 CCHO + #.046 RCHO + #.618 ACET + #.096 MEK + #.002 PROD2 + #.34 XC
3-Methyl Hexane [LP]	7.17e-12	7.17e-12			3-ME-C6 + HO. = #.75 RO2-R. + #.25 RO2-N. + #.924 R2O2. + #.002 HCHO + #.208 CCHO + #.463 RCHO + #.256 MEK + #.235 PROD2 + #1.266 XC
3-Methyl Hexane [AP]	7.17e-12	7.17e-12			3-ME-C6 + HO. = #.75 RO2-R. + #.25 RO2-N. + #.924 R2O2. + #.002 HCHO + #.208 CCHO + #.255 RCHO + #.256 MEK + #1.266 XC + #.235 PRD1 + #.208 PRD2
	1.65e-11	1.65e-11			PRD1 + HO. = #.409 HO2. + #.454 RO2-R. + #.065 RO2-N. + #.07 CCO-O2. + #.001 RCO-O2. + #.055 HCHO + #.312 CCHO + #.232 RCHO + #.215 MEK + #.486 PROD2 + #.311 XC
	PF=KETONE QY = 1.5e-2				PRD1 + HV = #.904 RO2-R. + #.096 RO2-N. + #.74 R2O2. + CCO-O2. + #.319 HCHO + #.542 CCHO + #.381 RCHO + #.251 PROD2 + #-0.629 XC
	2.32e-11	2.32e-11			PRD2 + HO. = #.128 RO2-R. + #.024 RO2-N. + #.022 R2O2. + #.848 RCO-O2. + #.011 CO + #.062 CCHO + #.128 RCHO + #.054 MEK + #.001 MGLY + #-0.423 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.017 HCHO + #.766 CCHO + #.032 RCHO + #.783 PROD2 + #-5.454 XC
2,2,3,3-Tetrame. Butane [LP]	1.05e-12	1.72e-12	0.29	2.0	2233M-C4 + HO. = #.067 RO2-R. + #.316 RO2-N. + #2.106 R2O2. + #.617 TBU-O. + #.761 HCHO + #.059 RCHO + #.659 ACET + #1.337 XC
2,2,3,3-Tetrame. Butane [AP]	1.05e-12	1.72e-12	0.29	2.0	2233M-C4 + HO. = #.067 RO2-R. + #.316 RO2-N. + #2.106 R2O2. + #.617 TBU-O. + #.761 HCHO + #.659 ACET + #1.337 XC + #.059 PRD1
	2.41e-11	2.41e-11			PRD1 + HO. = #.145 HO2. + #.041 RO2-R. + #.007 RO2-N. + #.807 RCO-O2. + #.005 CO + #.017 HCHO + #.179 RCHO + #.006 ACET + #.005 MEK + #.001 PROD2 + #.002 MGLY + #-0.072 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.135 HO2. + #1.643 RO2-R. + #.222 RO2-N. + CO + #.778 HCHO + #1.643 ACET + #-5.038 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
2,2,4-Trimethyl Pentane [LP]	3.56e-12	1.87e-12	-0.39	2.0	224TM-C5 + HO. = #.403 RO2-R. + #.227 RO2-N. + #1.961 R2O2. + #.37 TBU-O. + #.717 HCHO + #.002 CCHO + #.388 RCHO + #.38 ACET + #.133 MEK + #.027 PROD2 + #1.809 XC
2,2,4-Trimethyl Pentane [AP]	3.56e-12	1.87e-12	-0.39	2.0	224TM-C5 + HO. = #.403 RO2-R. + #.227 RO2-N. + #1.961 R2O2. + #.37 TBU-O. + #.717 HCHO + #.002 CCHO + #.38 ACET + #.133 MEK + #.027 PROD2 + #1.809 XC + #.388 PRD1
	2.49e-11	2.49e-11			PRD1 + HO. = #.081 RO2-R. + #.01 RO2-N. + #.021 R2O2. + #.906 RCO-O2. + #.004 TBU-O. + #.064 CO + #.014 HCHO + #.008 CCHO + #.021 RCHO + #.059 ACET + #.008 MEK + #.001 PROD2 + #-0.154 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.735 HO2. + #1.189 RO2-R. + #.074 RO2-N. + #.003 TBU-O. + CO + #.177 HCHO + #.004 CCHO + #.856 ACET + #.094 MEK + #.061 PROD2 + #-1.947 XC
2,2-Dimethyl Hexane [LP]	4.80e-12	4.80e-12			22-DM-C6 + HO. = #.457 RO2-R. + #.29 RO2-N. + #.953 R2O2. + #.253 TBU-O. + #.035 HCHO + #.041 CCHO + #.367 RCHO + #.001 ACET + #.013 MEK + #.341 PROD2 + #2.183 XC
2,2-Dimethyl Hexane [AP]	4.80e-12	4.80e-12			22-DM-C6 + HO. = #.457 RO2-R. + #.29 RO2-N. + #.953 R2O2. + #.253 TBU-O. + #.035 HCHO + #.041 CCHO + #.012 RCHO + #.001 ACET + #.013 MEK + #2.183 XC + #.355 PRD1 + #.341 PRD2
	2.52e-11	2.52e-11			PRD1 + HO. = #.058 HO2. + #.091 RO2-R. + #.01 RO2-N. + #.012 R2O2. + #.842 RCO-O2. + #.047 CO + #.012 HCHO + #.018 CCHO + #.138 RCHO + #.006 ACET + #.001 GLY + #-0.11 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.825 HO2. + #1.109 RO2-R. + #.066 RO2-N. + CO + #.011 HCHO + #.141 CCHO + #.934 RCHO + #.012 ACET + #-1.526 XC
	6.31e-12	6.31e-12			PRD2 + HO. = #.161 HO2. + #.212 RO2-R. + #.14 RO2-N. + #.714 R2O2. + #.077 CCO-O2. + #.123 RCO-O2. + #.287 TBU-O. + #.084 HCHO + #.046 CCHO + #.788 RCHO + #.021 ACET + #.019 MEK + #1.096 XC
		PF=KETONE QY = 4.8e-3			PRD2 + HV = #.818 RO2-R. + #.182 RO2-N. + #.907 R2O2. + CCO-O2. + #.087 HCHO + #.006 CCHO + #.786 RCHO + #.033 ACET + #.354 XC
2,3,4-Trimethyl Pentane	7.10e-12	7.10e-12			234TM-C5 + HO. = #.717 RO2-R. + #.283 RO2-N. + #1.284 R2O2. + #.039 HCHO + #.447 CCHO + #.033 RCHO + #1.141 ACET + #.296 MEK + #.664 XC
2,3-Dimethyl Hexane [LP]	8.57e-12	8.57e-12			23-DM-C6 + HO. = #.7 RO2-R. + #.3 RO2-N. + #1.143 R2O2. + #.014 HCHO + #.128 CCHO + #.184 RCHO + #.561 ACET + #.299 MEK + #.25 PROD2 + XC
2,3-Dimethyl Hexane [AP]	8.57e-12	8.57e-12			23-DM-C6 + HO. = #.7 RO2-R. + #.3 RO2-N. + #1.143 R2O2. + #.014 HCHO + #.128 CCHO + #.184 RCHO + #.561 ACET + #.299 MEK + XC + #.25 PRD1
	1.10e-11	1.10e-11			PRD1 + HO. = #.211 HO2. + #.613 RO2-R. + #.093 RO2-N. + #.034 R2O2. + #.078 CCO-O2. + #.006 RCO-O2. + #.263 HCHO + #.004 CCHO + #.584 RCHO + #.311 ACET + #.302 MEK + #.011 PROD2 + #1.039 XC
		PF=KETONE QY = 2.7e-2			PRD1 + HV = RO2-R. + #.013 R2O2. + CCO-O2. + #.033 HCHO + #.002 CCHO + #.987 RCHO + XC
2,4-Dimethyl Hexane [LP]	8.57e-12	8.57e-12			24-DM-C6 + HO. = #.652 RO2-R. + #.348 RO2-N. + #1.346 R2O2. + #.159 HCHO + #.335 CCHO + #.306 RCHO + #.096 ACET + #.156 MEK + #.293 PROD2 + #1.492 XC
2,4-Dimethyl Hexane [AP]	8.57e-12	8.57e-12			24-DM-C6 + HO. = #.652 RO2-R. + #.348 RO2-N. + #1.346 R2O2. + #.159 HCHO + #.335 CCHO + #.096 ACET + #.156 MEK + #1.492 XC + #.306 PRD1 + #.293 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.49e-11	2.49e-11			PRD1 + HO. = #.111 RO2-R. + #.015 RO2-N. + #.015 R2O2. + #.874 RCO-O2. + #.077 CO + #.006 HCHO + #.035 CCHO + #.034 RCHO + #.034 ACET + #.047 MEK + #-0.257 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.657 HO2. + #1.226 RO2-R. + #.117 RO2-N. + CO + #.003 HCHO + #.35 CCHO + #.494 ACET + #.085 MEK + #.248 PROD2 + #-2.716 XC
	1.40e-11	1.40e-11			PRD2 + HO. = #.488 HO2. + #.221 RO2-R. + #.068 RO2-N. + #.268 R2O2. + #.213 CCO-O2. + #.009 RCO-O2. + #.145 HCHO + #.003 CCHO + #.433 RCHO + #.22 ACET + #.398 MEK + #.011 PROD2 + #1.369 XC
		PF=KETONE QY = 2.4e-2			PRD2 + HV = #.968 RO2-R. + #.032 RO2-N. + #.049 R2O2. + CCO-O2. + #.884 HCHO + #.446 CCHO + #.087 RCHO + #.047 ACET + #.388 MEK + #.08 XC
2,5-Dimethyl Hexane [LP]	8.29e-12	8.29e-12			25-DM-C6 + HO. = #.649 RO2-R. + #.351 RO2-N. + #1.53 R2O2. + #.156 HCHO + #.434 RCHO + #.569 ACET + #.225 PROD2 + #1.378 XC
2,5-Dimethyl Hexane [AP]	8.29e-12	8.29e-12			25-DM-C6 + HO. = #.649 RO2-R. + #.351 RO2-N. + #1.53 R2O2. + #.156 HCHO + #.569 ACET + #1.378 XC + #.434 PRD1 + #.225 PRD2
	2.69e-11	2.69e-11			PRD1 + HO. = #.096 HO2. + #.09 RO2-R. + #.01 RO2-N. + #.048 R2O2. + #.001 C-O2. + #.803 RCO-O2. + #.058 CO + #.04 HCHO + #.131 RCHO + #.052 ACET + #.011 MEK + #.004 PROD2 + #.017 GLY + #-0.225 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.742 HO2. + #1.183 RO2-R. + #.075 RO2-N. + CO + #.575 HCHO + #.355 RCHO + #.317 ACET + #.346 MEK + #.001 PROD2 + #-2.434 XC
	1.47e-11	1.47e-11			PRD2 + HO. = #.634 HO2. + #.237 RO2-R. + #.042 RO2-N. + #.044 CCO-O2. + #.043 RCO-O2. + #.147 HCHO + #.053 CCHO + #.754 RCHO + #.021 ACET + #.13 MEK + #2.435 XC
		PF=KETONE QY = 7.1e-2			PRD2 + HV = RO2-R. + CCO-O2. + #1.611 HCHO + #.195 CCHO + #2 XC
2-Methyl Heptane [LP]	8.31e-12	8.31e-12			2-ME-C7 + HO. = #.659 RO2-R. + #.341 RO2-N. + #.882 R2O2. + #.016 HCHO + #.025 CCHO + #.155 RCHO + #.024 ACET + #.546 PROD2 + #2.077 XC
2-Methyl Heptane [AP]	8.31e-12	8.31e-12			2-ME-C7 + HO. = #.659 RO2-R. + #.341 RO2-N. + #.882 R2O2. + #.016 HCHO + #.025 CCHO + #.037 RCHO + #.024 ACET + #2.077 XC + #.118 PRD1 + #.546 PRD2
	2.92e-11	2.92e-11			PRD1 + HO. = #.129 HO2. + #.142 RO2-R. + #.025 RO2-N. + #.003 R2O2. + #.704 RCO-O2. + #.037 CO + #.007 HCHO + #.003 CCHO + #.294 RCHO + #.028 ACET + #.019 PROD2 + #.001 MGLY + #-0.394 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.146 HO2. + #1.664 RO2-R. + #.189 RO2-N. + CO + #.187 HCHO + #.945 RCHO + #.223 PROD2 + #-3.499 XC
	1.29e-11	1.29e-11			PRD2 + HO. = #.138 HO2. + #.556 RO2-R. + #.139 RO2-N. + #.129 R2O2. + #.008 CCO-O2. + #.159 RCO-O2. + #.112 HCHO + #.091 CCHO + #.552 RCHO + #.304 ACET + #.264 PROD2 + #.23 XC
3-Methyl Heptane [LP]	8.59e-12	8.59e-12			3-ME-C7 + HO. = #.662 RO2-R. + #.338 RO2-N. + #.942 R2O2. + #.001 HCHO + #.178 CCHO + #.15 RCHO + #.062 MEK + #.521 PROD2 + #1.788 XC
3-Methyl Heptane [AP]	8.59e-12	8.59e-12			3-ME-C7 + HO. = #.662 RO2-R. + #.338 RO2-N. + #.942 R2O2. + #.001 HCHO + #.178 CCHO + #.062 MEK + #1.788 XC + #.15 PRD1 + #.521 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	1.20e-11	1.20e-11			PRD2 + HO. = #.202 HO2. + #.569 RO2-R. + #.133 RO2-N. + #.079 R2O2. + #.075 CCO-O2. + #.022 RCO-O2. + #.018 HCHO + #.181 CCHO + #.52 RCHO + #.394 MEK + #.286 PROD2 + #-0.241 XC
		PF=KETONE QY = 6.7e-3			PRD2 + HV = RO2-R. + CCO-O2. + #1.611 HCHO + #.195 CCHO + #2 XC
4-Methyl Heptane [LP]	8.59e-12	8.59e-12			4-ME-C7 + HO. = #.676 RO2-R. + #.324 RO2-N. + #.875 R2O2. + #.002 HCHO + #.004 CCHO + #.377 RCHO + #.115 MEK + #.376 PROD2 + #2.201 XC
4-Methyl Heptane [AP]	8.59e-12	8.59e-12			4-ME-C7 + HO. = #.676 RO2-R. + #.324 RO2-N. + #.875 R2O2. + #.002 HCHO + #.004 CCHO + #.193 RCHO + #.115 MEK + #2.201 XC + #.184 PRD1 + #.376 PRD2
	2.46e-11	2.46e-11			PRD1 + HO. = #.156 RO2-R. + #.046 RO2-N. + #.062 R2O2. + #.798 RCO-O2. + #.008 CO + #.001 HCHO + #.221 RCHO + #.049 MEK + #.032 PROD2 + #.001 MGLY + #-0.729 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.133 HO2. + #1.614 RO2-R. + #.252 RO2-N. + CO + #.011 HCHO + #.737 RCHO + #.724 PROD2 + #-6.08 XC
	1.80e-11	1.80e-11			PRD2 + HO. = #.393 HO2. + #.444 RO2-R. + #.082 RO2-N. + #.028 CCO-O2. + #.054 RCO-O2. + #.07 HCHO + #.123 CCHO + #.439 RCHO + #.158 MEK + #.463 PROD2 + #.244 XC
		PF=KETONE QY = 7.7e-3			PRD2 + HV = RO2-R. + #.013 R2O2. + CCO-O2. + #.033 HCHO + #.002 CCHO + #.987 RCHO + XC
2,2,5-Trimethyl Hexane [LP]	6.08e-12	6.08e-12			225TM-C6 + HO. = #.475 RO2-R. + #.33 RO2-N. + #1.307 R2O2. + #.195 TBU-O. + #.046 HCHO + #.002 CCHO + #.613 RCHO + #.433 ACET + #.004 MEK + #.056 PROD2 + #2.899 XC
2,2,5-Trimethyl Hexane [AP]	6.08e-12	6.08e-12			225TM-C6 + HO. = #.475 RO2-R. + #.33 RO2-N. + #1.307 R2O2. + #.195 TBU-O. + #.046 HCHO + #.002 CCHO + #.433 ACET + #.004 MEK + #2.899 XC + #.613 PRD1 + #.056 PRD2
	2.53e-11	2.53e-11			PRD1 + HO. = #.075 HO2. + #.084 RO2-R. + #.011 RO2-N. + #.044 R2O2. + #.001 C-O2. + #.828 RCO-O2. + #.001 TBU-O. + #.057 CO + #.045 HCHO + #.125 RCHO + #.042 ACET + #.008 GLY + #-0.17 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.242 HO2. + #1.442 RO2-R. + #.121 RO2-N. + #.179 R2O2. + #.195 TBU-O. + CO + #1.018 HCHO + #.246 RCHO + #.488 ACET + #-2.533 XC
	7.93e-12	7.93e-12			PRD2 + HO. = #.059 HO2. + #.503 RO2-R. + #.122 RO2-N. + #.315 RCO-O2. + #.177 HCHO + #.064 CCHO + #.623 RCHO + #.164 ACET + #.029 MEK + #1.543 XC
2,3,5-Trimethyl Hexane [LP]	7.90e-12	7.90e-12			235TM-C6 + HO. = #.622 RO2-R. + #.378 RO2-N. + #1.356 R2O2. + #.094 HCHO + #.104 CCHO + #.178 RCHO + #.63 ACET + #.017 MEK + #.436 PROD2 + #1.327 XC
2,3,5-Trimethyl Hexane [AP]	7.90e-12	7.90e-12			235TM-C6 + HO. = #.622 RO2-R. + #.378 RO2-N. + #1.356 R2O2. + #.094 HCHO + #.104 CCHO + #.63 ACET + #.017 MEK + #1.327 XC + #.436 PRD1 + #.178 PRD2
	1.40e-11	1.40e-11			PRD1 + HO. = #.222 HO2. + #.172 RO2-R. + #.073 RO2-N. + #.946 R2O2. + #.525 CCO-O2. + #.009 RCO-O2. + #.599 HCHO + #.013 CCHO + #.263 RCHO + #.426 ACET + #.216 MEK + #.931 XC
		PF=KETONE QY = 3.8e-2			PRD1 + HV = #.952 RO2-R. + #.048 RO2-N. + #.342 R2O2. + CCO-O2. + #.727 HCHO + #.232 CCHO + #.383 RCHO + #.185 ACET + #.152 MEK + #.211 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.60e-11	2.60e-11			PRD2 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
2,4-Dimethyl Heptane [LP]	9.99e-12	9.99e-12			24-DM-C7 + HO. = #.598 RO2-R. + #.402 RO2-N. + #1.176 R2O2. + #.104 HCHO + #.013 CCHO + #.41 RCHO + #.049 ACET + #.073 MEK + #.381 PROD2 + #2.501 XC
2,4-Dimethyl Heptane [AP]	9.99e-12	9.99e-12			24-DM-C7 + HO. = #.598 RO2-R. + #.402 RO2-N. + #1.176 R2O2. + #.104 HCHO + #.013 CCHO + #.215 RCHO + #.049 ACET + #.073 MEK + #2.501 XC + #.196 PRD1 + #.381 PRD2
	2.59e-11	2.59e-11			PRD1 + HO. = #.142 RO2-R. + #.042 RO2-N. + #.05 R2O2. + #.815 RCO-O2. + #.047 CO + #.007 HCHO + #.004 CCHO + #.132 RCHO + #.025 ACET + #.049 MEK + #.024 PROD2 + #-0.57 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.47 HO2. + #1.313 RO2-R. + #.217 RO2-N. + CO + #.005 HCHO + #.428 RCHO + #.346 ACET + #.428 PROD2 + #-4.197 XC
	1.60e-11	1.60e-11			PRD2 + HO. = #.384 HO2. + #.308 RO2-R. + #.1 RO2-N. + #.219 R2O2. + #.112 CCO-O2. + #.095 RCO-O2. + #.112 HCHO + #.056 CCHO + #.394 RCHO + #.179 ACET + #.274 MEK + #.191 PROD2 + #.705 XC
		PF=KETONE QY = 1.4e-2			PRD2 + HV = #.966 RO2-R. + #.034 RO2-N. + #.07 R2O2. + CCO-O2. + #.846 HCHO + #.377 CCHO + #.123 RCHO + #.067 ACET + #.399 MEK + #.03 XC
2-Methyl Octane [LP]	1.01e-11	1.01e-11			2-ME-C8 + HO. = #.587 RO2-R. + #.413 RO2-N. + #.914 R2O2. + #.002 HCHO + #.064 RCHO + #.014 ACET + #.536 PROD2 + #3.072 XC
2-Methyl Octane [AP]	1.01e-11	1.01e-11			2-ME-C8 + HO. = #.587 RO2-R. + #.413 RO2-N. + #.914 R2O2. + #.002 HCHO + #.064 RCHO + #.014 ACET + #3.072 XC + #.536 PRD1
	1.75e-11	1.75e-11			PRD1 + HO. = #.202 HO2. + #.499 RO2-R. + #.149 RO2-N. + #.103 R2O2. + #.001 C-O2. + #.008 CCO-O2. + #.141 RCO-O2. + #.104 HCHO + #.055 CCHO + #.544 RCHO + #.18 ACET + #.339 PROD2 + #.246 XC
3,3-Diethyl Pentane	4.90e-12	4.90e-12			33-DE-C5 + HO. = #.647 RO2-R. + #.353 RO2-N. + #1.45 R2O2. + #.053 HCHO + #1.321 CCHO + #.022 RCHO + #.607 MEK + #.018 PROD2 + #1.585 XC
3,5-Dimethyl Heptane [LP]	1.03e-11	1.03e-11			35-DM-C7 + HO. = #.549 RO2-R. + #.451 RO2-N. + #1.467 R2O2. + #.01 HCHO + #.648 CCHO + #.155 RCHO + #.075 MEK + #.399 PROD2 + #1.83 XC
3,5-Dimethyl Heptane [AP]	1.03e-11	1.03e-11			35-DM-C7 + HO. = #.549 RO2-R. + #.451 RO2-N. + #1.467 R2O2. + #.01 HCHO + #.648 CCHO + #.075 MEK + #1.83 XC + #.155 PRD1 + #.399 PRD2
	2.25e-11	2.25e-11			PRD1 + HO. = #.119 RO2-R. + #.014 RO2-N. + #.046 R2O2. + #.867 RCO-O2. + #.119 CO + #.09 CCHO + #.076 MEK + #-0.284 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.637 HO2. + #1.282 RO2-R. + #.08 RO2-N. + CO + #.725 CCHO + #.557 MEK + #-2.161 XC
	2.07e-11	2.07e-11			PRD2 + HO. = #.607 HO2. + #.218 RO2-R. + #.078 RO2-N. + #.101 R2O2. + #.093 CCO-O2. + #.003 RCO-O2. + #.026 HCHO + #.039 CCHO + #.189 RCHO + #.832 MEK + #.048 PROD2 + #1.049 XC
		PF=KETONE QY = 3.2e-2			PRD2 + HV = #.982 RO2-R. + #.018 RO2-N. + CCO-O2. + #.982 HCHO + #.982 CCHO + #.946 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
4-Ethyl Heptane [LP]	1.04e-11	1.04e-11			4-ET-C7 + HO. = #.633 RO2-R. + #.367 RO2-N. + #.862 R2O2. + #.001 HCHO + #.049 CCHO + #.328 RCHO + #.486 PROD2 + #2.799 XC
4-Ethyl Heptane [AP]	1.04e-11	1.04e-11			4-ET-C7 + HO. = #.633 RO2-R. + #.367 RO2-N. + #.862 R2O2. + #.001 HCHO + #.049 CCHO + #.182 RCHO + #2.799 XC + #.145 PRD1 + #.486 PRD2
	2.58e-11	2.58e-11			PRD1 + HO. = #.177 RO2-R. + #.061 RO2-N. + #.059 R2O2. + #.761 RCO-O2. + #.005 CO + #.056 CCHO + #.231 RCHO + #.061 PROD2 + #-0.832 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.173 HO2. + #1.51 RO2-R. + #.317 RO2-N. + CO + #.284 CCHO + #.399 RCHO + #.671 PROD2 + #-5.693 XC
	1.65e-11	1.65e-11			PRD2 + HO. = #.185 HO2. + #.495 RO2-R. + #.121 RO2-N. + #.207 R2O2. + #.021 CCO-O2. + #.179 RCO-O2. + #.078 HCHO + #.225 CCHO + #.323 RCHO + #.144 MEK + #.389 PROD2 + #.291 XC
		PF=KETONE QY = 1.5e-2			PRD2 + HV = #.984 RO2-R. + #.016 RO2-N. + #.003 R2O2. + RCO-O2. + #.007 HCHO + #.001 CCHO + #.982 RCHO + #-0.047 XC
4-Methyl Octane [LP]	9.70e-12	9.70e-12			4-ME-C8 + HO. = #.605 RO2-R. + #.395 RO2-N. + #.89 R2O2. + #.001 HCHO + #.034 CCHO + #.127 RCHO + #.006 MEK + #.562 PROD2 + #2.788 XC
4-Methyl Octane [AP]	9.70e-12	9.70e-12			4-ME-C8 + HO. = #.605 RO2-R. + #.395 RO2-N. + #.89 R2O2. + #.001 HCHO + #.034 CCHO + #.057 RCHO + #.006 MEK + #2.788 XC + #.562 PRD1 + #.07 PRD2
	1.60e-11	1.60e-11			PRD1 + HO. = #.193 HO2. + #.552 RO2-R. + #.165 RO2-N. + #.088 R2O2. + #.041 CCO-O2. + #.049 RCO-O2. + #.014 HCHO + #.048 CCHO + #.545 RCHO + #.287 MEK + #.401 PROD2 + #-0.517 XC
	2.33e-11	2.33e-11			PRD2 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
2,4-Dimethyl Octane [LP]	1.14e-11	1.14e-11			24-DM-C8 + HO. = #.555 RO2-R. + #.445 RO2-N. + #1.06 R2O2. + #.041 HCHO + #.034 CCHO + #.21 RCHO + #.024 ACET + #.007 MEK + #.49 PROD2 + #3.55 XC
2,4-Dimethyl Octane [AP]	1.14e-11	1.14e-11			24-DM-C8 + HO. = #.555 RO2-R. + #.445 RO2-N. + #1.06 R2O2. + #.041 HCHO + #.034 CCHO + #.024 ACET + #.007 MEK + #3.55 XC + #.49 PRD1 + #.21 PRD2
	1.47e-11	1.47e-11			PRD1 + HO. = #.218 HO2. + #.472 RO2-R. + #.188 RO2-N. + #.18 R2O2. + #.044 CCO-O2. + #.079 RCO-O2. + #.043 HCHO + #.024 CCHO + #.542 RCHO + #.061 ACET + #.199 MEK + #.355 PROD2 + #-0.276 XC
		PF=KETONE QY = 4.2e-3			PRD1 + HV = #.968 RO2-R. + #.032 RO2-N. + CCO-O2. + #.968 HCHO + #.361 CCHO + #.608 MEK + #-0.31 XC
	2.39e-11	2.39e-11			PRD2 + HO. = #.086 RO2-R. + #.007 RO2-N. + #.014 R2O2. + #.907 RCO-O2. + #.058 CO + #.014 HCHO + #.014 CCHO + #.057 RCHO + #.015 ACET + #-0.079 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.975 RO2-R. + #.025 RO2-N. + CO + #.757 RCHO + #.219 ACET + #-1.074 XC
2,6-Dimethyl Octane [LP]	1.29e-11	1.29e-11			26DM-C8 + HO. = #.567 RO2-R. + #.433 RO2-N. + #1.096 R2O2. + #.108 CCHO + #.308 RCHO + #.145 ACET + #.071 MEK + #.276 PROD2 + #3.887 XC
2,6-Dimethyl Octane [AP]	1.29e-11	1.29e-11			26DM-C8 + HO. = #.567 RO2-R. + #.433 RO2-N. + #1.096 R2O2. + #.108 CCHO + #.145 ACET + #.071 MEK + #3.887 XC + #.308 PRD1 + #.276 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.27e-11	2.27e-11			PRD1 + HO. = #.12 RO2-R. + #.019 RO2-N. + #.015 R2O2. + #.862 RCO-O2. + #.02 CO + #.007 HCHO + #.035 CCHO + #.118 RCHO + #.025 ACET + #.031 MEK + #.002 MGLY + #-0.352 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.124 HO2. + #1.719 RO2-R. + #.157 RO2-N. + CO + #.181 HCHO + #.433 CCHO + #.229 RCHO + #.614 PROD2 + #-4.362 XC
	1.71e-11	1.71e-11			PRD2 + HO. = #.049 HO2. + #.482 RO2-R. + #.221 RO2-N. + #.302 R2O2. + #.001 C-O2. + #.018 CCO-O2. + #.229 RCO-O2. + #.078 HCHO + #.22 CCHO + #.35 RCHO + #.163 ACET + #.142 MEK + #.304 PROD2 + #-0.501 XC
2-Methyl Nonane [LP]	1.28e-11	1.28e-11			2-ME-C9 + HO. = #.551 RO2-R. + #.449 RO2-N. + #.895 R2O2. + #.035 RCHO + #.012 ACET + #.516 PROD2 + #4.066 XC
2-Methyl Nonane [AP]	1.28e-11	1.28e-11			2-ME-C9 + HO. = #.551 RO2-R. + #.449 RO2-N. + #.895 R2O2. + #.035 RCHO + #.012 ACET + #4.066 XC + #.516 PRD1
	2.09e-11	2.09e-11			PRD1 + HO. = #.231 HO2. + #.495 RO2-R. + #.155 RO2-N. + #.053 R2O2. + #.001 C-O2. + #.006 CCO-O2. + #.112 RCO-O2. + #.044 HCHO + #.068 CCHO + #.48 RCHO + #.116 ACET + #.455 PROD2 + #.023 XC
3,4-Diethyl Hexane [LP]	7.40e-12	7.40e-12			34-DE-C6 + HO. = #.619 RO2-R. + #.381 RO2-N. + #1.105 R2O2. + #.007 HCHO + #.337 CCHO + #.319 RCHO + #.709 MEK + #.126 PROD2 + #2.483 XC
3,4-Diethyl Hexane [AP]	7.40e-12	7.40e-12			34-DE-C6 + HO. = #.619 RO2-R. + #.381 RO2-N. + #1.105 R2O2. + #.007 HCHO + #.337 CCHO + #.319 RCHO + #.709 MEK + #2.483 XC + #.126 PRD1
	2.74e-11	2.74e-11			PRD1 + HO. = #.125 HO2. + #.599 RO2-R. + #.174 RO2-N. + #.102 CCO-O2. + #.41 CCHO + #.054 RCHO + #.771 PROD2 + #-0.86 XC
3-Methyl Nonane [LP]	1.14e-11	1.14e-11			3-ME-C9 + HO. = #.551 RO2-R. + #.449 RO2-N. + #.928 R2O2. + #.036 CCHO + #.063 RCHO + #.014 MEK + #.502 PROD2 + #3.977 XC
3-Methyl Nonane [AP]	1.14e-11	1.14e-11			3-ME-C9 + HO. = #.551 RO2-R. + #.449 RO2-N. + #.928 R2O2. + #.036 CCHO + #.063 RCHO + #.014 MEK + #3.977 XC + #.502 PRD1
	1.94e-11	1.94e-11			PRD1 + HO. = #.167 HO2. + #.542 RO2-R. + #.172 RO2-N. + #.07 R2O2. + #.014 CCO-O2. + #.104 RCO-O2. + #.063 HCHO + #.128 CCHO + #.495 RCHO + #.13 MEK + #.392 PROD2 + #-0.049 XC
4-Methyl Nonane [LP]	1.14e-11	1.14e-11			4-ME-C9 + HO. = #.572 RO2-R. + #.428 RO2-N. + #.876 R2O2. + #.001 HCHO + #.019 CCHO + #.14 RCHO + #.004 MEK + #.52 PROD2 + #3.831 XC
4-Methyl Nonane [AP]	1.14e-11	1.14e-11			4-ME-C9 + HO. = #.572 RO2-R. + #.428 RO2-N. + #.876 R2O2. + #.001 HCHO + #.019 CCHO + #.14 RCHO + #.004 MEK + #3.831 XC + #.52 PRD1
	1.82e-11	1.82e-11			PRD1 + HO. = #.168 HO2. + #.541 RO2-R. + #.185 RO2-N. + #.091 R2O2. + #.009 CCO-O2. + #.098 RCO-O2. + #.009 HCHO + #.07 CCHO + #.525 RCHO + #.189 MEK + #.427 PROD2 + #-0.461 XC
4-Propyl Heptane [LP]	1.18e-11	1.18e-11			4-PR-C7 + HO. = #.593 RO2-R. + #.407 RO2-N. + #.834 R2O2. + #.001 HCHO + #.001 CCHO + #.296 RCHO + #.461 PROD2 + #3.899 XC
4-Propyl Heptane [AP]	1.18e-11	1.18e-11			4-PR-C7 + HO. = #.593 RO2-R. + #.407 RO2-N. + #.834 R2O2. + #.001 HCHO + #.001 CCHO + #.162 RCHO + #3.899 XC + #.134 PRD1 + #.461 PRD2
	2.72e-11	2.72e-11			PRD1 + HO. = #.202 RO2-R. + #.086 RO2-N. + #.087 R2O2. + #.712 RCO-O2. + #.004 CO + #.323 RCHO + #.066 PROD2 + #-1.022 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.206 HO2. + #1.423 RO2-R. + #.37 RO2-N. + CO + #.63 RCHO + #.62 PROD2 + #-5.828 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.02e-11	2.02e-11			PRD2 + HO. = #.169 HO2. + #.515 RO2-R. + #.15 RO2-N. + #.159 R2O2. + #.009 CCO-O2. + #.156 RCO-O2. + #.062 HCHO + #.127 CCHO + #.378 RCHO + #.572 PROD2 + #-0.27 XC
	PF=KETONE QY = 5.4e-3				PRD2 + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #-0.06 XC
2,6-Dimethyl Nonane [LP]	1.28e-11	1.28e-11			26DM-C9 + HO. = #.533 RO2-R. + #.467 RO2-N. + #1.036 R2O2. + #.001 CCHO + #.221 RCHO + #.12 ACET + #.006 MEK + #.376 PROD2 + #4.888 XC
2,6-Dimethyl Nonane [AP]	1.28e-11	1.28e-11			26DM-C9 + HO. = #.533 RO2-R. + #.467 RO2-N. + #1.036 R2O2. + #.001 CCHO + #.026 RCHO + #.12 ACET + #.006 MEK + #4.888 XC + #.195 PRD1 + #.376 PRD2
	2.41e-11	2.41e-11			PRD1 + HO. = #.147 RO2-R. + #.039 RO2-N. + #.05 R2O2. + #.814 RCO-O2. + #.013 CO + #.003 HCHO + #.198 RCHO + #.012 ACET + #.039 MEK + #.025 PROD2 + #.001 MGLY + #-0.635 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.139 HO2. + #1.636 RO2-R. + #.225 RO2-N. + CO + #.088 HCHO + #.687 RCHO + #.658 PROD2 + #-5.449 XC
	2.00e-11	2.00e-11			PRD2 + HO. = #.15 HO2. + #.498 RO2-R. + #.194 RO2-N. + #.151 R2O2. + #.001 C-O2. + #.011 CCO-O2. + #.147 RCO-O2. + #.076 HCHO + #.069 CCHO + #.481 RCHO + #.107 ACET + #.107 MEK + #.369 PROD2 + #-0.25 XC
	PF=KETONE QY = 3.9e-3				PRD2 + HV = RO2-R. + #.013 R2O2. + CCO-O2. + #.033 HCHO + #.002 CCHO + #.987 RCHO + XC
3,5-Diethyl Heptane [LP]	1.39e-11	1.39e-11			35-DE-C7 + HO. = #.465 RO2-R. + #.535 RO2-N. + #1.311 R2O2. + #.002 HCHO + #.475 CCHO + #.123 RCHO + #.044 MEK + #.371 PROD2 + #4.064 XC
3,5-Diethyl Heptane [AP]	1.39e-11	1.39e-11			35-DE-C7 + HO. = #.465 RO2-R. + #.535 RO2-N. + #1.311 R2O2. + #.002 HCHO + #.475 CCHO + #.023 RCHO + #.044 MEK + #4.064 XC + #.1 PRD1 + #.371 PRD2
	2.41e-11	2.41e-11			PRD1 + HO. = #.162 RO2-R. + #.032 RO2-N. + #.096 R2O2. + #.806 RCO-O2. + #.158 CO + #.082 CCHO + #.079 RCHO + #.082 MEK + #-0.5 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.625 HO2. + #1.259 RO2-R. + #.116 RO2-N. + CO + #.375 CCHO + #.375 RCHO + #.509 MEK + #-2.607 XC
	2.42e-11	2.42e-11			PRD2 + HO. = #.422 HO2. + #.248 RO2-R. + #.158 RO2-N. + #.278 R2O2. + #.152 CCO-O2. + #.019 RCO-O2. + #.201 CCHO + #.259 RCHO + #.64 MEK + #.075 PROD2 + #.501 XC
	PF=KETONE QY = 4.9e-3				PRD2 + HV = #.968 RO2-R. + #.032 RO2-N. + #.017 R2O2. + RCO-O2. + #.952 HCHO + #.968 RCHO + #-1.047 XC
3-Methyl Decane [LP]	1.29e-11	1.29e-11			3-ME-C10 + HO. = #.526 RO2-R. + #.474 RO2-N. + #.917 R2O2. + #.029 CCHO + #.038 RCHO + #.012 MEK + #.489 PROD2 + #4.998 XC
3-Methyl Decane [AP]	1.29e-11	1.29e-11			3-ME-C10 + HO. = #.526 RO2-R. + #.474 RO2-N. + #.917 R2O2. + #.029 CCHO + #.038 RCHO + #.012 MEK + #4.998 XC + #.489 PRD1
	2.26e-11	2.26e-11			PRD1 + HO. = #.196 HO2. + #.532 RO2-R. + #.175 RO2-N. + #.041 R2O2. + #.01 CCO-O2. + #.087 RCO-O2. + #.015 HCHO + #.131 CCHO + #.428 RCHO + #.087 MEK + #.487 PROD2 + #-0.168 XC
4-Methyl Decane [LP]	1.29e-11	1.29e-11			4-ME-C10 + HO. = #.531 RO2-R. + #.469 RO2-N. + #.907 R2O2. + #.001 CCHO + #.08 RCHO + #.003 MEK + #.5 PROD2 + #4.932 XC
4-Methyl Decane [AP]	1.29e-11	1.29e-11			4-ME-C10 + HO. = #.531 RO2-R. + #.469 RO2-N. + #.907 R2O2. + #.001 CCHO + #.08 RCHO + #.003 MEK + #4.932 XC + #.5 PRD1
	2.14e-11	2.14e-11			PRD1 + HO. = #.158 HO2. + #.551 RO2-R. + #.194 RO2-N. + #.068 R2O2. + #.007 CCO-O2. + #.09 RCO-O2. + #.047 HCHO + #.042 CCHO + #.533 RCHO + #.129 MEK + #.411 PROD2 + #-0.167 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
2,6-Diethyl Octane [LP]	1.53e-11	1.53e-11			36-DE-C8 + HO. = #.518 RO2-R. + #.482 RO2-N. + #1.155 R2O2. + #.301 CCHO + #.058 RCHO + #.108 MEK + #.473 PROD2 + #5.062 XC
2,6-Diethyl Octane [AP]	1.53e-11	1.53e-11			36-DE-C8 + HO. = #.518 RO2-R. + #.482 RO2-N. + #1.155 R2O2. + #.301 CCHO + #.058 RCHO + #.108 MEK + #5.062 XC + #.473 PRD1
	1.85e-11	1.85e-11			PRD1 + HO. = #.17 HO2. + #.518 RO2-R. + #.187 RO2-N. + #.098 R2O2. + #.018 CCO-O2. + #.109 RCO-O2. + #.218 CCHO + #.496 RCHO + #.196 MEK + #.318 PROD2 + #-0.097 XC
	PF=KETONE QY = 7.6e-3				PRD1 + HV = RO2-R. + RCO-O2. + #1.611 HCHO + #.195 CCHO + XC
3,6-Dimethyl Decane [LP]	1.45e-11	1.45e-11			36DM-C10 + HO. = #.494 RO2-R. + #.506 RO2-N. + #1.079 R2O2. + #.001 HCHO + #.088 CCHO + #.11 RCHO + #.055 MEK + #.458 PROD2 + #5.488 XC
3,6-Dimethyl Decane [AP]	1.45e-11	1.45e-11			36DM-C10 + HO. = #.494 RO2-R. + #.506 RO2-N. + #1.079 R2O2. + #.001 HCHO + #.088 CCHO + #.055 MEK + #5.488 XC + #.11 PRD1 + #.458 PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	1.90e-11	1.90e-11			PRD2 + HO. = #.162 HO2. + #.545 RO2-R. + #.208 RO2-N. + #.125 R2O2. + #.038 CCO-O2. + #.047 RCO-O2. + #.015 HCHO + #.079 CCHO + #.536 RCHO + #.088 MEK + #.516 PROD2 + #-0.697 XC
	PF=KETONE QY = 1.1e-2				PRD2 + HV = RO2-R. + CCO-O2. + #1.611 HCHO + #.195 CCHO + #2 XC
3-Methyl Undecane [LP]	1.43e-11	1.43e-11			3-ME-C11 + HO. = #.516 RO2-R. + #.484 RO2-N. + #.896 R2O2. + #.025 CCHO + #.033 RCHO + #.011 MEK + #.484 PROD2 + #5.997 XC
3-Methyl Undecane [AP]	1.43e-11	1.43e-11			3-ME-C11 + HO. = #.516 RO2-R. + #.484 RO2-N. + #.896 R2O2. + #.025 CCHO + #.033 RCHO + #.011 MEK + #5.997 XC + #.484 PRD1
	2.44e-11	2.44e-11			PRD1 + HO. = #.175 HO2. + #.542 RO2-R. + #.193 RO2-N. + #.049 R2O2. + #.012 CCO-O2. + #.078 RCO-O2. + #.012 HCHO + #.071 CCHO + #.46 RCHO + #.071 MEK + #.486 PROD2 + #-0.147 XC
5-Methyl Undecane [LP]	1.43e-11	1.43e-11			5-ME-C11 + HO. = #.524 RO2-R. + #.476 RO2-N. + #.867 R2O2. + #.01 CCHO + #.059 RCHO + #.504 PROD2 + #5.923 XC
5-Methyl Undecane [AP]	1.43e-11	1.43e-11			5-ME-C11 + HO. = #.524 RO2-R. + #.476 RO2-N. + #.867 R2O2. + #.01 CCHO + #.059 RCHO + #5.923 XC + #.504 PRD1
	2.09e-11	2.09e-11			PRD1 + HO. = #.12 HO2. + #.567 RO2-R. + #.237 RO2-N. + #.133 R2O2. + #.014 CCO-O2. + #.061 RCO-O2. + #.03 HCHO + #.023 CCHO + #.501 RCHO + #.035 MEK + #.537 PROD2 + #-0.579 XC
3,6-Dimethyl Undecane [LP]	1.60e-11	1.60e-11			36DM-C11 + HO. = #.488 RO2-R. + #.512 RO2-N. + #1.046 R2O2. + #.001 HCHO + #.07 CCHO + #.124 RCHO + #.046 MEK + #.442 PROD2 + #6.579 XC
3,6-Dimethyl Undecane [AP]	1.60e-11	1.60e-11			36DM-C11 + HO. = #.488 RO2-R. + #.512 RO2-N. + #1.046 R2O2. + #.001 HCHO + #.07 CCHO + #.02 RCHO + #.046 MEK + #6.579 XC + #.104 PRD1 + #.442 PRD2
	2.82e-11	2.82e-11			PRD1 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.96e-11	1.96e-11			PRD2 + HO. = #.145 HO2. + #.546 RO2-R. + #.229 RO2-N. + #.151 R2O2. + #.022 CCO-O2. + #.057 RCO-O2. + #.009 HCHO + #.077 CCHO + #.542 RCHO + #.039 MEK + #.531 PROD2 + #-0.722 XC
		PF=KETONE QY = 1.1e-2			PRD2 + HV = RO2-R. + CCO-O2. + #1.611 HCHO + #.195 CCHO + #2 XC
3,7-Diethyl Nonane [LP]	1.68e-11	1.68e-11			37-DE-C9 + HO. = #.5 RO2-R. + #.5 RO2-N. + #1.107 R2O2. + #.132 CCHO + #.293 RCHO + #.105 MEK + #.304 PROD2 + #6.607 XC
3,7-Diethyl Nonane [AP]	1.68e-11	1.68e-11			37-DE-C9 + HO. = #.5 RO2-R. + #.5 RO2-N. + #1.107 R2O2. + #.132 CCHO + #.075 RCHO + #.105 MEK + #6.607 XC + #.219 PRD1 + #.304 PRD2
	2.43e-11	2.43e-11			PRD1 + HO. = #.163 RO2-R. + #.042 RO2-N. + #.035 R2O2. + #.795 RCO-O2. + #.006 CO + #.102 CCHO + #.162 RCHO + #.049 MEK + #.006 PROD2 + #-0.563 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.135 HO2. + #1.613 RO2-R. + #.252 RO2-N. + CO + #.734 CCHO + #.014 RCHO + #.734 PROD2 + #-5.424 XC
	2.56e-11	2.56e-11			PRD2 + HO. = #.084 HO2. + #.504 RO2-R. + #.247 RO2-N. + #.243 R2O2. + #.023 CCO-O2. + #.143 RCO-O2. + #.021 HCHO + #.23 CCHO + #.427 RCHO + #.118 MEK + #.387 PROD2 + #-0.514 XC
3-Methyl Dodecane [LP]	1.57e-11	1.57e-11			3-ME-C12 + HO. = #.51 RO2-R. + #.49 RO2-N. + #.88 R2O2. + #.023 CCHO + #.03 RCHO + #.009 MEK + #.482 PROD2 + #6.997 XC
3-Methyl Dodecane [AP]	1.57e-11	1.57e-11			3-ME-C12 + HO. = #.51 RO2-R. + #.49 RO2-N. + #.88 R2O2. + #.023 CCHO + #.03 RCHO + #.009 MEK + #6.997 XC + #.482 PRD1
	2.58e-11	2.58e-11			PRD1 + HO. = #.117 HO2. + #.582 RO2-R. + #.218 RO2-N. + #.055 R2O2. + #.009 CCO-O2. + #.074 RCO-O2. + #.009 HCHO + #.058 CCHO + #.426 RCHO + #.061 MEK + #.491 PROD2 + #-0.14 XC
5-Methyl Dodecane [LP]	1.57e-11	1.57e-11			5-ME-C12 + HO. = #.514 RO2-R. + #.486 RO2-N. + #.863 R2O2. + #.009 CCHO + #.044 RCHO + #.498 PROD2 + #6.942 XC
5-Methyl Dodecane [AP]	1.57e-11	1.57e-11			5-ME-C12 + HO. = #.514 RO2-R. + #.486 RO2-N. + #.863 R2O2. + #.009 CCHO + #.044 RCHO + #6.942 XC + #.498 PRD1
	2.30e-11	2.30e-11			PRD1 + HO. = #.117 HO2. + #.572 RO2-R. + #.243 RO2-N. + #.125 R2O2. + #.012 CCO-O2. + #.055 RCO-O2. + #.009 HCHO + #.042 CCHO + #.433 RCHO + #.034 MEK + #.552 PROD2 + #-0.488 XC
3,7-Dimethyl Dodecane [LP]	1.74e-11	1.74e-11			37DM-C12 + HO. = #.496 RO2-R. + #.504 RO2-N. + #.98 R2O2. + #.055 CCHO + #.11 RCHO + #.03 MEK + #.44 PROD2 + #7.772 XC
3,7-Dimethyl Dodecane [AP]	1.74e-11	1.74e-11			37DM-C12 + HO. = #.496 RO2-R. + #.504 RO2-N. + #.98 R2O2. + #.055 CCHO + #.009 RCHO + #.03 MEK + #7.772 XC + #.101 PRD1 + #.44 PRD2
	2.74e-11	2.74e-11			PRD1 + HO. = #.197 RO2-R. + #.089 RO2-N. + #.111 R2O2. + #.714 RCO-O2. + #.007 CO + #.001 HCHO + #.005 CCHO + #.282 RCHO + #.075 PROD2 + #.001 MGLY + #-0.993 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.204 HO2. + #1.425 RO2-R. + #.371 RO2-N. + CO + #.009 HCHO + #.621 RCHO + #.607 PROD2 + #-5.736 XC
	2.28e-11	2.28e-11			PRD2 + HO. = #.075 HO2. + #.538 RO2-R. + #.276 RO2-N. + #.256 R2O2. + #.009 CCO-O2. + #.103 RCO-O2. + #.005 HCHO + #.093 CCHO + #.461 RCHO + #.064 MEK + #.498 PROD2 + #-0.795 XC
3,8-Diethyl Decane [LP]	1.82e-11	1.82e-11			38DE-C10 + HO. = #.471 RO2-R. + #.529 RO2-N. + #1.03 R2O2. + #.066 CCHO + #.057 RCHO + #.017 MEK + #.428 PROD2 + #7.885 XC
3,8-Diethyl Decane [AP]	1.82e-11	1.82e-11			38DE-C10 + HO. = #.471 RO2-R. + #.529 RO2-N. + #1.03 R2O2. + #.066 CCHO + #.01 RCHO + #.017 MEK + #7.885 XC + #.046 PRD1 + #.428 PRD2
	2.92e-11	2.92e-11			PRD1 + HO. = #.185 RO2-R. + #.126 RO2-N. + #.285 R2O2. + #.689 RCO-O2. + #.075 CO + #.023 CCHO + #.174 RCHO + #.007 MEK + #.016 MGLY + #-0.54 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.173 HO2. + #1.51 RO2-R. + #.317 RO2-N. + CO + #.683 RCHO + #-1.95 XC
	2.97e-11	2.97e-11			PRD2 + HO. = #.115 HO2. + #.573 RO2-R. + #.226 RO2-N. + #.115 R2O2. + #.013 CCO-O2. + #.072 RCO-O2. + #.009 HCHO + #.295 CCHO + #.286 RCHO + #.107 MEK + #.537 PROD2 + #-0.704 XC
3-Methyl Tridecane [LP]	1.71e-11	1.71e-11			3-ME-C13 + HO. = #.506 RO2-R. + #.494 RO2-N. + #.871 R2O2. + #.021 CCHO + #.015 RCHO + #.009 MEK + #.493 PROD2 + #7.958 XC
3-Methyl Tridecane [AP]	1.71e-11	1.71e-11			3-ME-C13 + HO. = #.506 RO2-R. + #.494 RO2-N. + #.871 R2O2. + #.021 CCHO + #.015 RCHO + #.009 MEK + #7.958 XC + #.493 PRD1
	2.65e-11	2.65e-11			PRD1 + HO. = #.087 HO2. + #.6 RO2-R. + #.238 RO2-N. + #.065 R2O2. + #.01 CCO-O2. + #.065 RCO-O2. + #.004 HCHO + #.045 CCHO + #.386 RCHO + #.06 MEK + #.496 PROD2 + #-0.109 XC
6-Methyl Tridecane [LP]	1.71e-11	1.71e-11			6-ME-C13 + HO. = #.512 RO2-R. + #.488 RO2-N. + #.852 R2O2. + #.006 CCHO + #.041 RCHO + #.504 PROD2 + #7.909 XC
6-Methyl Tridecane [AP]	1.71e-11	1.71e-11			6-ME-C13 + HO. = #.512 RO2-R. + #.488 RO2-N. + #.852 R2O2. + #.006 CCHO + #.041 RCHO + #7.909 XC + #.504 PRD1
	2.42e-11	2.42e-11			PRD1 + HO. = #.079 HO2. + #.596 RO2-R. + #.26 RO2-N. + #.137 R2O2. + #.006 CCO-O2. + #.059 RCO-O2. + #.008 HCHO + #.043 CCHO + #.429 RCHO + #.567 PROD2 + #-0.531 XC
3,7-Dimethyl Tridecane [LP]	1.88e-11	1.88e-11			37DM-C13 + HO. = #.487 RO2-R. + #.513 RO2-N. + #.98 R2O2. + #.045 CCHO + #.087 RCHO + #.028 MEK + #.44 PROD2 + #8.82 XC
3,7-Dimethyl Tridecane [AP]	1.88e-11	1.88e-11			37DM-C13 + HO. = #.487 RO2-R. + #.513 RO2-N. + #.98 R2O2. + #.045 CCHO + #.002 RCHO + #.028 MEK + #8.82 XC + #.085 PRD1 + #.44 PRD2
	2.89e-11	2.89e-11			PRD1 + HO. = #.205 RO2-R. + #.117 RO2-N. + #.159 R2O2. + #.678 RCO-O2. + #.006 CO + #.284 RCHO + #.056 PROD2 + #.001 MGLY + #-0.936 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.228 HO2. + #1.364 RO2-R. + #.408 RO2-N. + CO + #.008 HCHO + #.584 RCHO + #.571 PROD2 + #-5.634 XC
	2.41e-11	2.41e-11			PRD2 + HO. = #.05 HO2. + #.545 RO2-R. + #.288 RO2-N. + #.267 R2O2. + #.004 CCO-O2. + #.112 RCO-O2. + #.007 HCHO + #.093 CCHO + #.426 RCHO + #.066 MEK + #.472 PROD2 + #-0.644 XC
3,9-Diethyl Undecane [LP]	1.96e-11	1.96e-11			39DE-C11 + HO. = #.474 RO2-R. + #.526 RO2-N. + #.997 R2O2. + #.058 CCHO + #.051 RCHO + #.016 MEK + #.435 PROD2 + #8.899 XC
3,9-Diethyl Undecane [AP]	1.96e-11	1.96e-11			39DE-C11 + HO. = #.474 RO2-R. + #.526 RO2-N. + #.997 R2O2. + #.058 CCHO + #.051 RCHO + #.016 MEK + #8.899 XC + #.435 PRD1
	2.59e-11	2.59e-11			PRD1 + HO. = #.631 RO2-R. + #.269 RO2-N. + #.154 R2O2. + #.019 CCO-O2. + #.081 RCO-O2. + #.003 HCHO + #.185 CCHO + #.442 RCHO + #.202 MEK + #.373 PROD2 + #-0.641 XC
3-Methyl Tetradecane [LP]	1.85e-11	1.85e-11			3-ME-C14 + HO. = #.505 RO2-R. + #.495 RO2-N. + #.861 R2O2. + #.02 CCHO + #.013 RCHO + #.008 MEK + #.493 PROD2 + #8.961 XC
3-Methyl Tetradecane [AP]	1.85e-11	1.85e-11			3-ME-C14 + HO. = #.505 RO2-R. + #.495 RO2-N. + #.861 R2O2. + #.02 CCHO + #.013 RCHO + #.008 MEK + #8.961 XC + #.493 PRD1
	2.79e-11	2.79e-11			PRD1 + HO. = #.065 HO2. + #.615 RO2-R. + #.253 RO2-N. + #.085 R2O2. + #.004 CCO-O2. + #.063 RCO-O2. + #.004 HCHO + #.047 CCHO + #.363 RCHO + #.062 MEK + #.492 PROD2 + #-0.101 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
6-Methyl Tetradecane [LP]	1.85e-11	1.85e-11			6-ME-C14 + HO. = #.51 RO2-R. + #.49 RO2-N. + #.843 R2O2. + #.006 CCHO + #.037 RCHO + #.503 PROD2 + #8.918 XC
6-Methyl Tetradecane [AP]	1.85e-11	1.85e-11			6-ME-C14 + HO. = #.51 RO2-R. + #.49 RO2-N. + #.843 R2O2. + #.006 CCHO + #.037 RCHO + #8.918 XC + #.503 PRD1
	2.59e-11	2.59e-11			PRD1 + HO. = #.054 HO2. + #.61 RO2-R. + #.274 RO2-N. + #.149 R2O2. + #.007 CCO-O2. + #.055 RCO-O2. + #.006 HCHO + #.021 CCHO + #.411 RCHO + #.56 PROD2 + #-0.465 XC
3-Methyl Pentadecane [LP]	2.00e-11	2.00e-11			3-ME-C15 + HO. = #.504 RO2-R. + #.496 RO2-N. + #.853 R2O2. + #.018 CCHO + #.012 RCHO + #.008 MEK + #.493 PROD2 + #9.964 XC
3-Methyl Pentadecane [AP]	2.00e-11	2.00e-11			3-ME-C15 + HO. = #.504 RO2-R. + #.496 RO2-N. + #.853 R2O2. + #.018 CCHO + #.012 RCHO + #.008 MEK + #9.964 XC + #.493 PRD1
	2.93e-11	2.93e-11			PRD1 + HO. = #.043 HO2. + #.627 RO2-R. + #.267 RO2-N. + #.104 R2O2. + #.004 CCO-O2. + #.059 RCO-O2. + #.004 HCHO + #.045 CCHO + #.346 RCHO + #.058 MEK + #.491 PROD2 + #-0.095 XC
4,8-Dimethyl Tetradecane [LP]	2.02e-11	2.02e-11			48DM-C14 + HO. = #.481 RO2-R. + #.519 RO2-N. + #.962 R2O2. + #.001 CCHO + #.071 RCHO + #.003 MEK + #.473 PROD2 + #9.82 XC
4,8-Dimethyl Tetradecane [AP]	2.02e-11	2.02e-11			48DM-C14 + HO. = #.481 RO2-R. + #.519 RO2-N. + #.962 R2O2. + #.001 CCHO + #.071 RCHO + #.003 MEK + #9.82 XC + #.473 PRD1
	2.78e-11	2.78e-11			PRD1 + HO. = #.047 HO2. + #.619 RO2-R. + #.264 RO2-N. + #.109 R2O2. + #.004 CCO-O2. + #.066 RCO-O2. + #.005 HCHO + #.033 CCHO + #.425 RCHO + #.025 MEK + #.539 PROD2 + #-0.474 XC
7-Methyl Pentadecane [LP]	2.00e-11	2.00e-11			7-ME-C15 + HO. = #.503 RO2-R. + #.497 RO2-N. + #.853 R2O2. + #.022 RCHO + #.5 PROD2 + #9.95 XC
7-Methyl Pentadecane [AP]	2.00e-11	2.00e-11			7-ME-C15 + HO. = #.503 RO2-R. + #.497 RO2-N. + #.853 R2O2. + #.022 RCHO + #9.95 XC + #.5 PRD1
	2.85e-11	2.85e-11			PRD1 + HO. = #.038 HO2. + #.636 RO2-R. + #.269 RO2-N. + #.098 R2O2. + #.008 CCO-O2. + #.049 RCO-O2. + #.007 HCHO + #.02 CCHO + #.383 RCHO + #.546 PROD2 + #-0.251 XC
Cyclopropane [LP]	8.40e-14	8.40e-14			CYCC3 + HO. = #.949 RO2-R. + #.051 RO2-N. + #.949 R2O2. + #.949 RCHO + #-0.153 XC
Cyclopropane [AP]	8.40e-14	8.40e-14			CYCC3 + HO. = #.949 RO2-R. + #.051 RO2-N. + #.949 R2O2. + #-0.153 XC + #.949 PRD1
	3.90e-11	3.90e-11			PRD1 + HO. = #.013 RO2-R. + #.001 RO2-N. + #.986 RCO-O2. + #.011 CO + #.011 GLY + #.002 MGLY + #-0.002 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + #1.957 CO + #.957 HCHO + #.043 GLY
Cyclobutane	1.50e-12	1.50e-12			CYCC4 + HO. = #.117 RO2-N. + #1.803 R2O2. + #.883 RCO-O2. + #.65 XC
Cyclopentane [LP]	5.02e-12	2.31e-12	-0.47	2.0	CYCC5 + HO. = #.776 RO2-R. + #.224 RO2-N. + #1.661 R2O2. + #.054 CO + #.756 RCHO + #.02 MEK + #1.255 XC
Cyclopentane [AP]	5.02e-12	2.31e-12	-0.47	2.0	CYCC5 + HO. = #.776 RO2-R. + #.224 RO2-N. + #1.661 R2O2. + #.054 CO + #.02 MEK + #1.255 XC + #.756 PRD1
	4.56e-11	4.56e-11			PRD1 + HO. = #.123 HO2. + #.049 RO2-R. + #.003 RO2-N. + #.826 RCO-O2. + #.007 CO + #.004 HCHO + #.048 RCHO + #.026 GLY + #.123 MGLY + #-0.073 XC
	7.32e-15	7.32e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #1.017 HO2. + #.519 RO2-R. + #.018 RO2-N. + #.445 RCO-O2. + CO + #.002 HCHO + #.535 RCHO + #-1.055 XC
Cyclohexane [LP]	7.21e-12	2.59e-12	-0.61	2.0	CYCC6 + HO. = #.799 RO2-R. + #.201 RO2-N. + #.473 R2O2. + #.203 RCHO + #.597 PROD2 + #.608 XC
Cyclohexane [AP]	7.21e-12	2.59e-12	-0.61	2.0	CYCC6 + HO. = #.799 RO2-R. + #.201 RO2-N. + #.473 R2O2. + #.608 XC + #.597 PRD1 + #.203 PRD2
	6.39e-12	6.39e-12			PRD1 + HO. = #.386 RO2-R. + #.178 RO2-N. + #.722 R2O2. + #.436 RCO-O2. + #.059 HCHO + #.194 RCHO + #.197 PROD2 + #1.802 XC
		PF=KETONE QY = 5.0e-2			PRD1 + HV = #6 XC
	5.19e-11	5.19e-11			PRD2 + HO. = #.18 HO2. + #.07 RO2-R. + #.008 RO2-N. + #.743 RCO-O2. + #.01 CO + #.26 RCHO + #.004 GLY + #.014 MGLY + #-0.116 XC
	7.60e-15	7.60e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.437 HO2. + #1.462 RO2-R. + #.101 RO2-N. + #1.021 CO + #.365 HCHO + #.899 RCHO + #-1.691 XC
Isopropyl Cyclopropane [LP]	2.70e-12	2.70e-12			IPR-CC3 + HO. = #.833 RO2-R. + #.164 RO2-N. + #1.821 R2O2. + #.002 RCO-O2. + #.087 HCHO + #.087 CCHO + #.835 RCHO + #.77 ACET + #-0.068 XC
Isopropyl Cyclopropane [AP]	2.70e-12	2.70e-12			IPR-CC3 + HO. = #.833 RO2-R. + #.164 RO2-N. + #1.821 R2O2. + #.002 RCO-O2. + #.087 HCHO + #.087 CCHO + #.77 ACET + #-0.068 XC + #.835 PRD1
	3.90e-11	3.90e-11			PRD1 + HO. = #.013 RO2-R. + #.001 RO2-N. + #.986 RCO-O2. + #.011 CO + #.011 GLY + #.002 MGLY + #-0.002 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + #1.957 CO + #.957 HCHO + #.043 GLY
Methylcyclo-pentane [LP]	5.68e-12	5.68e-12			ME-CYCC5 + HO. = #.453 RO2-R. + #.306 RO2-N. + #1.847 R2O2. + #.239 CCO-O2. + #.003 RCO-O2. + #.023 CO + #.017 HCHO + #.689 RCHO + #.003 PROD2 + #1.556 XC
Methylcylo-pentane [AP]	5.68e-12	5.68e-12			ME-CYCC5 + HO. = #.453 RO2-R. + #.306 RO2-N. + #1.847 R2O2. + #.239 CCO-O2. + #.003 RCO-O2. + #.023 CO + #.017 HCHO + #.003 PROD2 + #1.556 XC + #.689 PRD1
	3.44e-11	3.44e-11			PRD1 + HO. = #.147 HO2. + #.105 RO2-R. + #.009 RO2-N. + #.009 CCO-O2. + #.73 RCO-O2. + #.024 CO + #.021 HCHO + #.004 CCHO + #.158 RCHO + #.046 GLY + #.103 MGLY + #-0.189 XC
	4.98e-15	4.98e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #1.316 HO2. + #.53 RO2-R. + #.01 RO2-N. + #.144 RCO-O2. + CO + #.013 HCHO + #.002 CCHO + #.84 RCHO + #.001 GLY + #-1.032 XC
1,3-Dimeth. Cyclopentane [LP]	6.82e-12	6.82e-12			13DMCYC5 + HO. = #.275 RO2-R. + #.381 RO2-N. + #1.873 R2O2. + #.344 CCO-O2. + #.001 RCO-O2. + #.037 CO + #.028 HCHO + #.002 CCHO + #.584 RCHO + #.035 PROD2 + #1.999 XC
1,3-Dimeth. Cyclopentane [AP]	6.82e-12	6.82e-12			13DMCYC5 + HO. = #.275 RO2-R. + #.381 RO2-N. + #1.873 R2O2. + #.344 CCO-O2. + #.001 RCO-O2. + #.037 CO + #.028 HCHO + #.002 CCHO + #1.999 XC + #.584 PRD1 + #.035 PRD2
	2.93e-11	2.93e-11			PRD1 + HO. = #.135 HO2. + #.162 RO2-R. + #.018 RO2-N. + #.003 R2O2. + #.009 CCO-O2. + #.675 RCO-O2. + #.025 CO + #.06 HCHO + #.002 CCHO + #.194 RCHO + #.057 MEK + #.009 PROD2 + #.057 GLY + #.058 MGLY + #-0.396 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.9 HO2. + #1.068 RO2-R. + #.032 RO2-N. + CO + #.857 HCHO + #.448 CCHO + #.368 RCHO + #.163 PROD2 + #-2.028 XC
	1.41e-11	1.41e-11			PRD2 + HO. = #.539 HO2. + #.363 RO2-R. + #.039 RO2-N. + #.058 CCO-O2. + #.009 HCHO + #.294 CCHO + #.361 RCHO + #.6 PROD2 + #.369 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=KETONE QY = 2.0e-2				PRD2 + HV = #.93 RO2-R. + #.07 RO2-N. + #.785 R2O2. + CCO-O2. + #.93 RCHO + #.789 XC
Cycloheptane [LP]	1.30e-11	1.30e-11			CYCC7 + HO. = #.509 RO2-R. + #.39 RO2-N. + #1.578 R2O2. + #.101 RCO-O2. + #.492 RCHO + #.017 PROD2 + #2.778 XC
Cycloheptane [AP]	1.30e-11	1.30e-11			CYCC7 + HO. = #.509 RO2-R. + #.39 RO2-N. + #1.578 R2O2. + #.101 RCO-O2. + #.017 PROD2 + #2.778 XC + #.492 PRD1
	5.34e-11	5.34e-11			PRD1 + HO. = #.171 HO2. + #.092 RO2-R. + #.014 RO2-N. + #.723 RCO-O2. + #.008 CO + #.326 RCHO + #-0.242 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #1.065 RCHO + #-2.308 XC
Ethyl Cyclo-pentane [LP]	7.27e-12	7.27e-12			ET-CYCC5 + HO. = #.404 RO2-R. + #.389 RO2-N. + #1.86 R2O2. + #.208 RCO-O2. + #.019 CO + #.007 HCHO + #.132 CCHO + #.59 RCHO + #.003 MEK + #.004 PROD2 + #.01 MGLY + #1.922 XC
Ethyl Cyclo-pentane [AP]	7.27e-12	7.27e-12			ET-CYCC5 + HO. = #.404 RO2-R. + #.389 RO2-N. + #1.86 R2O2. + #.208 RCO-O2. + #.019 CO + #.007 HCHO + #.132 CCHO + #.003 MEK + #.004 PROD2 + #.01 MGLY + #1.922 XC + #.59 PRD1
	3.50e-11	3.50e-11			PRD1 + HO. = #.139 HO2. + #.107 RO2-R. + #.012 RO2-N. + #.743 RCO-O2. + #.023 CO + #.022 HCHO + #.006 CCHO + #.158 RCHO + #.038 GLY + #.097 MGLY + #-0.194 XC
	5.07e-15	5.07e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #1.268 HO2. + #.564 RO2-R. + #.011 RO2-N. + #.156 RCO-O2. + CO + #.013 HCHO + #.001 CCHO + #.827 RCHO + #-1.034 XC
Methylcyclo-hexane [LP]	1.00e-11	1.00e-11			ME-CYCC6 + HO. = #.66 RO2-R. + #.34 RO2-N. + #1.146 R2O2. + #.011 HCHO + #.002 CCHO + #.455 RCHO + #.208 PROD2 + #2.328 XC
Methylcyclo-hexane [AP]	1.00e-11	1.00e-11			ME-CYCC6 + HO. = #.66 RO2-R. + #.34 RO2-N. + #1.146 R2O2. + #.011 HCHO + #.002 CCHO + #2.328 XC + #.455 PRD1 + #.208 PRD2
	4.72e-11	4.72e-11			PRD1 + HO. = #.374 HO2. + #.1 RO2-R. + #.016 RO2-N. + #.021 CCO-O2. + #.489 RCO-O2. + #.01 CO + #.545 RCHO + #.003 GLY + #.001 MGLY + #-0.256 XC
	4.39e-15	4.39e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.3 HO2. + #1.107 RO2-R. + #.154 RO2-N. + #.319 R2O2. + #.438 CCO-O2. + #1.014 CO + #.316 HCHO + #.001 CCHO + #.832 RCHO + #.013 PROD2 + #.001 GLY + #-2.715 XC
	1.57e-11	1.57e-11			PRD2 + HO. = #.513 RO2-R. + #.253 RO2-N. + #1.191 R2O2. + #.234 RCO-O2. + #.179 HCHO + #.11 CCHO + #.508 RCHO + #.03 PROD2 + #.007 GLY + #1.66 XC
	PF=KETONE QY = 2.0e-2				PRD2 + HV = #5.405 XC
1,3-Dimethyl Cyclohexane [LP]	1.19e-11	1.19e-11			13DMCYC6 + HO. = #.553 RO2-R. + #.445 RO2-N. + #1.397 R2O2. + #.001 CCO-O2. + #.009 CO + #.02 HCHO + #.014 CCHO + #.509 RCHO + #.001 MEK + #.059 PROD2 + #3.389 XC
1,3-Dimethyl Cyclohexane [AP]	1.19e-11	1.19e-11			13DMCYC6 + HO. = #.553 RO2-R. + #.445 RO2-N. + #1.397 R2O2. + #.001 CCO-O2. + #.009 CO + #.02 HCHO + #.014 CCHO + #.001 MEK + #3.389 XC + #.509 PRD1 + #.059 PRD2
	4.52e-11	4.52e-11			PRD1 + HO. = #.336 HO2. + #.112 RO2-R. + #.025 RO2-N. + #.009 R2O2. + #.02 CCO-O2. + #.506 RCO-O2. + #.021 CO + #.001 CCHO + #.476 RCHO + #.047 MEK + #.015 PROD2 + #.004 GLY + #-0.449 XC
	4.10e-15	4.10e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.338 HO2. + #1.008 RO2-R. + #.211 RO2-N. + #.344 R2O2. + #.443 CCO-O2. + #1.003 CO + #.213 HCHO + #.099 CCHO + #.756 RCHO + #.033 PROD2 + #.021 GLY + #-3.074 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.19e-11	2.19e-11			PRD2 + HO. = #.368 RO2-R. + #.373 RO2-N. + #1.573 R2O2. + #.014 CCO-O2. + #.245 RCO-O2. + #.574 HCHO + #.109 CCHO + #.143 RCHO + #.23 MEK + #.024 MGLY + #.784 XC
	PF=KETONE QY = 1.0e-2				PRD2 + HV = #6 XC
Cyclooctane [LP]	1.40e-11	1.40e-11			CYCC8 + HO. = #.525 RO2-R. + #.475 RO2-N. + #1.475 R2O2. + #.001 CO + #.525 RCHO + #3.573 XC
Cyclooctane [AP]	1.40e-11	1.40e-11			CYCC8 + HO. = #.525 RO2-R. + #.475 RO2-N. + #1.475 R2O2. + #.001 CO + #3.573 XC + #.525 PRD1
	5.37e-11	5.37e-11			PRD1 + HO. = #.159 HO2. + #.124 RO2-R. + #.026 RO2-N. + #.69 RCO-O2. + #.004 CO + #.007 HCHO + #.337 RCHO + #.007 GLY + #.012 MGLY + #-0.297 XC
	7.32e-15	7.32e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.62 HO2. + #1.146 RO2-R. + #.179 RO2-N. + #.055 RCO-O2. + CO + #.791 RCHO + #-1.611 XC
Ethylcyclo-hexane [LP]	1.20e-11	1.20e-11			ET-CYCC6 + HO. = #.624 RO2-R. + #.376 RO2-N. + #1.046 R2O2. + #.002 HCHO + #.151 CCHO + #.328 RCHO + #.299 PROD2 + #2.662 XC
Ethylcyclo-hexane [AP]	1.20e-11	1.20e-11			ET-CYCC6 + HO. = #.624 RO2-R. + #.376 RO2-N. + #1.046 R2O2. + #.002 HCHO + #.151 CCHO + #.001 RCHO + #2.662 XC + #.299 PRD1 + #.327 PRD2
	1.33e-11	1.33e-11			PRD1 + HO. = #.471 RO2-R. + #.247 RO2-N. + #.948 R2O2. + #.282 RCO-O2. + #.076 HCHO + #.114 CCHO + #.353 RCHO + #.176 PROD2 + #.002 GLY + #1.243 XC
	PF=KETONE QY = 2.7e-2				PRD1 + HV = #5.66 XC
	4.80e-11	4.80e-11			PRD2 + HO. = #.351 HO2. + #.115 RO2-R. + #.024 RO2-N. + #.51 RCO-O2. + #.01 CO + #.012 CCHO + #.534 RCHO + #.003 GLY + #.001 MGLY + #-0.316 XC
	4.37e-15	4.37e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.32 HO2. + #1.076 RO2-R. + #.209 RO2-N. + #.263 R2O2. + #.395 RCO-O2. + #1.016 CO + #.311 HCHO + #.776 RCHO + #.015 PROD2 + #.001 GLY + #-3.189 XC
Propyl Cyclo-pentane [LP]	8.69e-12	8.69e-12			PR-CYCC5 + HO. = #.39 RO2-R. + #.458 RO2-N. + #1.739 R2O2. + #.152 RCO-O2. + #.013 CO + #.007 HCHO + #.001 CCHO + #.638 RCHO + #.002 MEK + #.027 PROD2 + #.005 MGLY + #2.677 XC
Propyl Cyclo-pentane [AP]	8.69e-12	8.69e-12			PR-CYCC5 + HO. = #.39 RO2-R. + #.458 RO2-N. + #1.739 R2O2. + #.152 RCO-O2. + #.013 CO + #.007 HCHO + #.001 CCHO + #.13 RCHO + #.002 MEK + #.027 PROD2 + #.005 MGLY + #2.677 XC + #.509 PRD1
	3.90e-11	3.90e-11			PRD1 + HO. = #.158 HO2. + #.12 RO2-R. + #.018 RO2-N. + #.704 RCO-O2. + #.019 CO + #.023 HCHO + #.007 CCHO + #.213 RCHO + #.034 GLY + #.081 MGLY + #-0.225 XC
	5.13e-15	5.13e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #1.219 HO2. + #.577 RO2-R. + #.024 RO2-N. + #.179 RCO-O2. + CO + #.012 HCHO + #.019 CCHO + #.792 RCHO + #-1.108 XC
1,1,3-Trimethyl Cyclohex. [LP]	8.70e-12	8.70e-12			113MCYC6 + HO. = #.484 RO2-R. + #.512 RO2-N. + #1.581 R2O2. + #.004 CCO-O2. + #.073 CO + #.132 HCHO + #.107 CCHO + #.473 RCHO + #.042 ACET + #.005 MEK + #.103 PROD2 + #3.318 XC
1,1,3-Trimethyl Cyclohex. [AP]	8.70e-12	8.70e-12			113MCYC6 + HO. = #.484 RO2-R. + #.512 RO2-N. + #1.581 R2O2. + #.004 CCO-O2. + #.073 CO + #.132 HCHO + #.107 CCHO + #.042 ACET + #.005 MEK + #3.318 XC + #.473 PRD1 + #.103 PRD2
	3.83e-11	3.83e-11			PRD1 + HO. = #.185 HO2. + #.044 RO2-R. + #.011 RO2-N. + #.029 R2O2. + #.015 CCO-O2. + #.745 RCO-O2. + #.015 CO + #.01 HCHO + #.243 RCHO + #.021 ACET + #.004 GLY + #.001 MGLY + #-0.161 XC
	5.10e-15	5.10e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.376 HO2. + #1.188 RO2-R. + #.164 RO2-N. + #.197 R2O2. + #.273 CCO-O2. + #1.328 CO + #.44 HCHO + #.409 RCHO + #.027 ACET + #.001 MEK + #.084 PROD2 + #.015 GLY + #-2.14 XC
	9.98e-12	9.98e-12			PRD2 + HO. = #.249 HO2. + #.082 RO2-R. + #.282 RO2-N. + #1.248 R2O2. + #.005 C-O2. + #.059 CCO-O2. + #.323 RCO-O2. + #.56 HCHO + #.002 CCHO + #.35 RCHO + #.231 ACET + #.045 MEK + #.006 MGLY + #.715 XC
		PF=KETONE QY = 3.9e-3			PRD2 + HV = #.961 RO2-R. + #.039 RO2-N. + CCO-O2. + #.961 HCHO + #.961 MEK + #-1.039 XC
1-Eth.-4-Meth. Cyclohex. [LP]	1.37e-11	1.37e-11			1E4MCYC6 + HO. = #.518 RO2-R. + #.481 RO2-N. + #1.339 R2O2. + #.001 CCO-O2. + #.033 HCHO + #.142 CCHO + #.411 RCHO + #.143 PROD2 + #3.703 XC
1-Eth.-4-Meth. Cyclohex. [AP]	1.37e-11	1.37e-11			1E4MCYC6 + HO. = #.518 RO2-R. + #.481 RO2-N. + #1.339 R2O2. + #.001 CCO-O2. + #.033 HCHO + #.142 CCHO + #.009 RCHO + #3.703 XC + #.143 PRD1 + #.403 PRD2
	1.38e-11	1.38e-11			PRD1 + HO. = #.572 RO2-R. + #.259 RO2-N. + #1.2 R2O2. + #.169 RCO-O2. + #.006 HCHO + #.208 CCHO + #.621 RCHO + #.002 PROD2 + #.009 GLY + #1.623 XC
		PF=KETONE QY = 2.0e-2			PRD1 + HV = #6 XC
	4.08e-11	4.08e-11			PRD2 + HO. = #.233 HO2. + #.141 RO2-R. + #.043 RO2-N. + #.026 R2O2. + #.014 CCO-O2. + #.569 RCO-O2. + #.003 CO + #.021 CCHO + #.485 RCHO + #.011 PROD2 + #.011 GLY + #-0.577 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.48 HO2. + #.97 RO2-R. + #.243 RO2-N. + #.193 R2O2. + #.15 CCO-O2. + #.157 RCO-O2. + CO + #.441 HCHO + #.01 CCHO + #.343 RCHO + #.425 PROD2 + #-4.267 XC
Propyl Cyclo-hexane [LP]	1.34e-11	1.34e-11			C3-CYCC6 + HO. = #.61 RO2-R. + #.389 RO2-N. + #.864 R2O2. + #.001 RCO-O2. + #.001 HCHO + #.363 RCHO + #.388 PROD2 + #3.242 XC
Propyl Cyclo-hexane [AP]	1.34e-11	1.34e-11			C3-CYCC6 + HO. = #.61 RO2-R. + #.389 RO2-N. + #.864 R2O2. + #.001 RCO-O2. + #.001 HCHO + #.138 RCHO + #3.242 XC + #.388 PRD1 + #.225 PRD2
	1.87e-11	1.87e-11			PRD1 + HO. = #.03 HO2. + #.526 RO2-R. + #.242 RO2-N. + #.583 R2O2. + #.003 CCO-O2. + #.199 RCO-O2. + #.036 HCHO + #.037 CCHO + #.34 RCHO + #.31 PROD2 + #.954 XC
		PF=KETONE QY = 1.4e-2			PRD1 + HV = #6 XC
	4.07e-11	4.07e-11			PRD2 + HO. = #.177 HO2. + #.205 RO2-R. + #.065 RO2-N. + #.046 R2O2. + #.554 RCO-O2. + #.004 CO + #.018 HCHO + #.007 CCHO + #.426 RCHO + #.019 PROD2 + #.001 GLY + #-0.484 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.211 HO2. + #1.251 RO2-R. + #.295 RO2-N. + #.156 R2O2. + #.243 RCO-O2. + CO + #.121 HCHO + #.705 RCHO + #-2.736 XC
1,3-Diethyl-Cyclohexane [LP]	1.55e-11	1.55e-11			13DECYC6 + HO. = #.49 RO2-R. + #.51 RO2-N. + #1.249 R2O2. + #.004 CO + #.002 HCHO + #.176 CCHO + #.334 RCHO + #.001 MEK + #.165 PROD2 + #4.582 XC
1,3-Diethyl-Cyclohexane [AP]	1.55e-11	1.55e-11			13DECYC6 + HO. = #.49 RO2-R. + #.51 RO2-N. + #1.249 R2O2. + #.004 CO + #.002 HCHO + #.176 CCHO + #.005 RCHO + #.001 MEK + #4.582 XC + #.165 PRD1 + #.329 PRD2
	2.20e-11	2.20e-11			PRD1 + HO. = #.506 RO2-R. + #.322 RO2-N. + #1.136 R2O2. + #.173 RCO-O2. + #.164 HCHO + #.251 CCHO + #.311 RCHO + #.009 MEK + #.213 PROD2 + #.001 GLY + #.001 MGLY + #.632 XC
		PF=KETONE QY = 7.9e-3			PRD1 + HV = #5 XC
	4.75e-11	4.75e-11			PRD2 + HO. = #.309 HO2. + #.161 RO2-R. + #.051 RO2-N. + #.012 R2O2. + #.479 RCO-O2. + #.02 CO + #.05 CCHO + #.497 RCHO + #.035 MEK + #.018 PROD2 + #.001 GLY + #-0.598 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.338 HO2. + #1.013 RO2-R. + #.313 RO2-N. + #.194 R2O2. + #.336 RCO-O2. + CO + #.101 HCHO + #.068 CCHO + #.641 RCHO + #.147 PROD2 + #-3.925 XC
1,4-Diethyl-Cyclohexane [LP]	1.55e-11	1.55e-11			14DECYC6 + HO. = #.508 RO2-R. + #.49 RO2-N. + #1.229 R2O2. + #.002 RCO-O2. + #.021 HCHO + #.226 CCHO + #.333 RCHO + #.209 PROD2 + #4.328 XC
1,4-Diethyl-Cyclohexane [AP]	1.55e-11	1.55e-11			14DECYC6 + HO. = #.508 RO2-R. + #.49 RO2-N. + #1.229 R2O2. + #.002 RCO-O2. + #.021 HCHO + #.226 CCHO + #.013 RCHO + #4.328 XC + #.209 PRD1 + #.32 PRD2
	1.56e-11	1.56e-11			PRD1 + HO. = #.537 RO2-R. + #.319 RO2-N. + #1.172 R2O2. + #.144 RCO-O2. + #.001 HCHO + #.116 CCHO + #.696 RCHO + #.051 PROD2 + #.007 GLY + #1.01 XC
		PF=KETONE QY = 1.0e-2			PRD1 + HV = #6 XC
	4.34e-11	4.34e-11			PRD2 + HO. = #.183 HO2. + #.137 RO2-R. + #.05 RO2-N. + #.033 R2O2. + #.63 RCO-O2. + #.003 CO + #.036 CCHO + #.422 RCHO + #.007 PROD2 + #.007 GLY + #-0.585 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.465 HO2. + #.947 RO2-R. + #.254 RO2-N. + #.122 R2O2. + #.335 RCO-O2. + CO + #.506 HCHO + #.264 RCHO + #.392 PROD2 + #-4.175 XC
1-Meth.-3-Isopr. Cyclohex. [LP]	1.51e-11	1.51e-11			1M3IPCY6 + HO. = #.535 RO2-R. + #.46 RO2-N. + #1.204 R2O2. + #.004 RCO-O2. + #.006 CO + #.008 HCHO + #.005 CCHO + #.263 RCHO + #.339 ACET + #.293 PROD2 + #3.634 XC
1-Meth.-3-Isopr. Cyclohex. [AP]	1.51e-11	1.51e-11			1M3IPCY6 + HO. = #.535 RO2-R. + #.46 RO2-N. + #1.204 R2O2. + #.004 RCO-O2. + #.006 CO + #.008 HCHO + #.005 CCHO + #.339 ACET + #3.634 XC + #.293 PRD1 + #.263 PRD2
	1.81e-11	1.81e-11			PRD1 + HO. = #.478 RO2-R. + #.264 RO2-N. + #1.186 R2O2. + #.258 RCO-O2. + #.283 HCHO + #.04 CCHO + #.406 RCHO + #.054 ACET + #.081 PROD2 + #.006 GLY + #1.401 XC
		PF=KETONE QY = 1.8e-2			PRD1 + HV = #5 XC
	5.31e-11	5.31e-11			PRD2 + HO. = #.335 HO2. + #.14 RO2-R. + #.038 RO2-N. + #.007 CCO-O2. + #.48 RCO-O2. + #.025 CO + #.004 HCHO + #.003 CCHO + #.488 RCHO + #.01 ACET + #.045 MEK + #.013 PROD2 + #.003 GLY + #.001 MGLY + #-0.476 XC
	4.76e-15	4.76e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.342 HO2. + #1.153 RO2-R. + #.261 RO2-N. + #.133 R2O2. + #.231 CCO-O2. + #.013 RCO-O2. + #1.023 CO + #.274 HCHO + #.001 CCHO + #.721 RCHO + #.083 ACET + #.022 PROD2 + #.002 GLY + #-2.912 XC
Butyl Cyclo-hexane [LP]	1.49e-11	1.49e-11			C4-CYCC6 + HO. = #.576 RO2-R. + #.423 RO2-N. + #.827 R2O2. + #.024 CCHO + #.179 RCHO + #.467 PROD2 + #4.07 XC
Butyl Cyclo-hexane [AP]	1.49e-11	1.49e-11			C4-CYCC6 + HO. = #.576 RO2-R. + #.423 RO2-N. + #.827 R2O2. + #.024 CCHO + #4.07 XC + #.467 PRD1 + #.179 PRD2
	1.94e-11	1.94e-11			PRD1 + HO. = #.031 HO2. + #.577 RO2-R. + #.278 RO2-N. + #.424 R2O2. + #.019 CCO-O2. + #.094 RCO-O2. + #.031 HCHO + #.017 CCHO + #.399 RCHO + #.386 PROD2 + #.432 XC
		PF=KETONE QY = 4.6e-3			PRD1 + HV = #6 XC
	2.33e-11	2.33e-11			PRD2 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
13-Dieth-5-Me. Cyclohex. [LP]	1.72e-11	1.72e-11			13E5MCC6 + HO. = #.429 RO2-R. + #.566 RO2-N. + #1.371 R2O2. + #.003 CCO-O2. + #.002 RCO-O2. + #.006 CO + #.02 HCHO + #.168 CCHO + #.355 RCHO + #.009 MEK + #.09 PROD2 + #5.587 XC
13-Dieth-5-Me. Cyclohex. [AP]	1.72e-11	1.72e-11			13E5MCC6 + HO. = #.429 RO2-R. + #.566 RO2-N. + #1.371 R2O2. + #.003 CCO-O2. + #.002 RCO-O2. + #.006 CO + #.02 HCHO + #.168 CCHO + #.007 RCHO + #.009 MEK + #5.587 XC + #.09 PRD1 + #.348 PRD2
	2.52e-11	2.52e-11			PRD1 + HO. = #.392 RO2-R. + #.422 RO2-N. + #1.438 R2O2. + #.002 CCO-O2. + #.184 RCO-O2. + #.372 HCHO + #.181 CCHO + #.228 RCHO + #.115 MEK + #.075 PROD2 + #.001 GLY + #.011 MGLY + #.545 XC
	2.65e-11	2.65e-11			PRD2 + HO. = #.14 RO2-R. + #.072 RO2-N. + #.086 R2O2. + #.01 CCO-O2. + #.778 RCO-O2. + #.059 CO + #.063 CCHO + #.119 RCHO + #.094 MEK + #.002 MGLY + #-0.713 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + #-0 XC + XN PRD2 + HV = #.009 HO2. + #1.273 RO2-R. + #.406 RO2-N. + #.088 R2O2. + #.065 CCO-O2. + #.247 RCO-O2. + CO + #.01 HCHO + #.237 CCHO + #.316 RCHO + #.006 MEK + #.275 PROD2 + #.024 MGLY + #-4.49 XC
1-Ethyl-2-Propyl Cyclohex. [LP]	1.70e-11	1.70e-11			1E2PCYC6 + HO. = #.461 RO2-R. + #.539 RO2-N. + #1.199 R2O2. + #.001 RCO-O2. + #.007 HCHO + #.031 CCHO + #.186 RCHO + #.349 PROD2 + #5.045 XC
1-Ethyl-2-Propyl Cyclohex. [AP]	1.70e-11	1.70e-11			1E2PCYC6 + HO. = #.461 RO2-R. + #.539 RO2-N. + #1.199 R2O2. + #.001 RCO-O2. + #.007 HCHO + #.031 CCHO + #.186 RCHO + #5.045 XC + #.349 PRD1
	3.90e-11	3.90e-11			PRD1 + HO. = #.451 HO2. + #.276 RO2-R. + #.192 RO2-N. + #.359 R2O2. + #.082 RCO-O2. + #.014 HCHO + #.039 CCHO + #.273 RCHO + #.613 PROD2 + #.001 GLY + #.001 MGLY + #.01 XC
Pentyl Cyclo-hexane [LP]	1.63e-11	1.63e-11			C5-CYCC6 + HO. = #.557 RO2-R. + #.443 RO2-N. + #.808 R2O2. + #.016 CCHO + #.147 RCHO + #.456 PROD2 + #5.135 XC
Pentyl Cyclo-hexane [AP]	1.63e-11	1.63e-11			C5-CYCC6 + HO. = #.557 RO2-R. + #.443 RO2-N. + #.808 R2O2. + #.016 CCHO + #.147 RCHO + #5.135 XC + #.456 PRD1
	2.33e-11	2.33e-11			PRD1 + HO. = #.03 HO2. + #.574 RO2-R. + #.295 RO2-N. + #.356 R2O2. + #.003 CCO-O2. + #.098 RCO-O2. + #.022 HCHO + #.029 CCHO + #.403 RCHO + #.404 PROD2 + #.219 XC
1,3,5-Triethyl Cyclohex. [LP]	1.90e-11	1.90e-11			135ECYC6 + HO. = #.417 RO2-R. + #.58 RO2-N. + #1.353 R2O2. + #.003 RCO-O2. + #.005 CO + #.014 HCHO + #.221 CCHO + #.315 RCHO + #.008 MEK + #.116 PROD2 + #6.373 XC
1,3,5-Triethyl Cyclohex. [AP]	1.90e-11	1.90e-11			135ECYC6 + HO. = #.417 RO2-R. + #.58 RO2-N. + #1.353 R2O2. + #.003 RCO-O2. + #.005 CO + #.014 HCHO + #.221 CCHO + #.007 RCHO + #.008 MEK + #6.373 XC + #.116 PRD1 + #.308 PRD2
	2.85e-11	2.85e-11			PRD1 + HO. = #.41 RO2-R. + #.454 RO2-N. + #1.345 R2O2. + #.136 RCO-O2. + #.222 HCHO + #.232 CCHO + #.281 RCHO + #.044 MEK + #.128 PROD2 + #.004 MGLY + #.384 XC
	3.45e-11	3.45e-11			PRD2 + HO. = #.03 HO2. + #.194 RO2-R. + #.089 RO2-N. + #.075 R2O2. + #.687 RCO-O2. + #.047 CO + #.097 CCHO + #.215 RCHO + #.05 MEK + #.039 PROD2 + #.001 GLY + #.003 MGLY + #-0.928 XC
	4.20e-15	4.20e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.322 HO2. + #1.169 RO2-R. + #.372 RO2-N. + #.136 RCO-O2. + #1.004 CO + #.034 HCHO + #.239 CCHO + #.411 RCHO + #.319 PROD2 + #.001 GLY + #.012 MGLY + #-4.345 XC
1-Meth.-4-Pentyl Cyclo-hexane	1.80e-11	1.80e-11			1M4C5CY6 + HO. = #.482 RO2-R. + #.518 RO2-N. + #1.049 R2O2. + #.001 CCO-O2. + #.001 HCHO + #.015 CCHO + #.21 RCHO + #.326 PROD2 + #6.274 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Hexyl Cyclo-hexane [LP]	1.78e-11	1.78e-11			C6-CYCC6 + HO. = #.527 RO2-R. + #.473 RO2-N. + #.849 R2O2. + #.093 RCHO + #.461 PROD2 + #6.118 XC
Hexyl Cyclo-hexane [AP]	1.78e-11	1.78e-11			C6-CYCC6 + HO. = #.527 RO2-R. + #.473 RO2-N. + #.849 R2O2. + #.093 RCHO + #6.118 XC + #.461 PRD1
	2.61e-11	2.61e-11			PRD1 + HO. = #.036 HO2. + #.574 RO2-R. + #.298 RO2-N. + #.313 R2O2. + #.003 CCO-O2. + #.089 RCO-O2. + #.042 HCHO + #.013 CCHO + #.407 RCHO + #.396 PROD2 + #.271 XC
13-Dieth-5-Pent Cyclohx. [LP]	2.05e-11	2.05e-11			13E5PCC6 + HO. = #.433 RO2-R. + #.564 RO2-N. + #1.237 R2O2. + #.003 RCO-O2. + #.002 CO + #.01 HCHO + #.132 CCHO + #.342 RCHO + #.002 MEK + #.188 PROD2 + #7.163 XC
13-Dieth-5-Pent Cyclohx. [AP]	2.05e-11	2.05e-11			13E5PCC6 + HO. = #.433 RO2-R. + #.564 RO2-N. + #1.237 R2O2. + #.003 RCO-O2. + #.002 CO + #.01 HCHO + #.132 CCHO + #.087 RCHO + #.002 MEK + #7.163 XC + #.188 PRD1 + #.255 PRD2
	3.14e-11	3.14e-11			PRD1 + HO. = #.441 RO2-R. + #.404 RO2-N. + #.953 R2O2. + #.154 RCO-O2. + #.108 HCHO + #.182 CCHO + #.281 RCHO + #.013 MEK + #.23 PROD2 + #.002 MGLY + #.36 XC
	2.98e-11	2.98e-11			PRD2 + HO. = #.169 RO2-R. + #.11 RO2-N. + #.147 R2O2. + #.721 RCO-O2. + #.054 CO + #.005 HCHO + #.064 CCHO + #.192 RCHO + #.017 MEK + #.077 PROD2 + #.002 MGLY + #-1.118 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.068 HO2. + #1.3 RO2-R. + #.445 RO2-N. + #.186 RCO-O2. + CO + #.204 CCHO + #.326 RCHO + #.369 PROD2 + #.016 MGLY + #-4.873 XC
1-Meth.-2-Hexyl-Cyclo-hexane [LP]	1.94e-11	1.94e-11			1M2C6CC6 + HO. = #.462 RO2-R. + #.537 RO2-N. + #1.08 R2O2. + #.001 RCO-O2. + #.004 HCHO + #.009 CCHO + #.128 RCHO + #.38 PROD2 + #7.092 XC
1-Meth.-2-Hexyl-Cyclo-hexane [AP]	1.94e-11	1.94e-11			1M2C6CC6 + HO. = #.462 RO2-R. + #.537 RO2-N. + #1.08 R2O2. + #.001 RCO-O2. + #.004 HCHO + #.009 CCHO + #.001 RCHO + #7.092 XC + #.38 PRD1 + #.126 PRD2
	3.46e-11	3.46e-11			PRD1 + HO. = #.196 HO2. + #.468 RO2-R. + #.27 RO2-N. + #.311 R2O2. + #.008 CCO-O2. + #.058 RCO-O2. + #.009 HCHO + #.035 CCHO + #.301 RCHO + #.534 PROD2 + #.003 XC
	2.43e-11	2.43e-11			PRD2 + HO. = #.112 RO2-R. + #.04 RO2-N. + #.154 R2O2. + #.848 RCO-O2. + #.014 CO + #.002 HCHO + #.103 RCHO + #.018 MGLY + #-0.166 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.874 RCHO + #-1.377 XC
Heptyl Cyclo-hexane [LP]	1.91e-11	1.91e-11			C7-CYCC6 + HO. = #.515 RO2-R. + #.485 RO2-N. + #.855 R2O2. + #.069 RCHO + #.462 PROD2 + #7.108 XC
Heptyl Cyclo-hexane [AP]	1.91e-11	1.91e-11			C7-CYCC6 + HO. = #.515 RO2-R. + #.485 RO2-N. + #.855 R2O2. + #.069 RCHO + #7.108 XC + #.462 PRD1
	2.87e-11	2.87e-11			PRD1 + HO. = #.06 HO2. + #.564 RO2-R. + #.295 RO2-N. + #.286 R2O2. + #.002 CCO-O2. + #.079 RCO-O2. + #.015 HCHO + #.034 CCHO + #.354 RCHO + #.448 PROD2 + #.154 XC
13-Diprop-5-Eth Cyclohx. [LP]	2.19e-11	2.19e-11			13P5ECC6 + HO. = #.445 RO2-R. + #.553 RO2-N. + #1.158 R2O2. + #.002 RCO-O2. + #.001 CO + #.007 HCHO + #.06 CCHO + #.376 RCHO + #.234 PROD2 + #8.017 XC
13-Diprop-5-Eth Cyclohx. [AP]	2.19e-11	2.19e-11			13P5ECC6 + HO. = #.445 RO2-R. + #.553 RO2-N. + #1.158 R2O2. + #.002 RCO-O2. + #.001 CO + #.007 HCHO + #.06 CCHO + #.154 RCHO + #8.017 XC + #.234 PRD1 + #.222 PRD2
	3.25e-11	3.25e-11			PRD1 + HO. = #.445 RO2-R. + #.417 RO2-N. + #.918 R2O2. + #.138 RCO-O2. + #.061 HCHO + #.106 CCHO + #.339 RCHO + #.249 PROD2 + #.001 MGLY + #.295 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.32e-11	3.32e-11			PRD2 + HO. = #.199 RO2-R. + #.152 RO2-N. + #.233 R2O2. + #.648 RCO-O2. + #.038 CO + #.013 HCHO + #.037 CCHO + #.256 RCHO + #.08 PROD2 + #.002 MGLY + #-1.235 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.132 HO2. + #1.286 RO2-R. + #.454 RO2-N. + #.128 RCO-O2. + CO + #.07 CCHO + #.456 RCHO + #.282 PROD2 + #.011 MGLY + #-4.342 XC
1-Meth.-4-Heptyl Cyclo-hexane	2.08e-11	2.08e-11			1M4C7CC6 + HO. = #.455 RO2-R. + #.544 RO2-N. + #1.059 R2O2. + #.001 HCHO + #.131 RCHO + #.349 PROD2 + #8.242 XC
Octyl Cyclo-hexane [LP]	2.05e-11	2.05e-11			C8-CYCC6 + HO. = #.511 RO2-R. + #.489 RO2-N. + #.847 R2O2. + #.063 RCHO + #.463 PROD2 + #8.099 XC
Octyl Cyclo-hexane [AP]	2.05e-11	2.05e-11			C8-CYCC6 + HO. = #.511 RO2-R. + #.489 RO2-N. + #.847 R2O2. + #.063 RCHO + #8.099 XC + #.463 PRD1
	2.99e-11	2.99e-11			PRD1 + HO. = #.058 HO2. + #.554 RO2-R. + #.311 RO2-N. + #.32 R2O2. + #.004 CCO-O2. + #.074 RCO-O2. + #.012 HCHO + #.01 CCHO + #.347 RCHO + #.454 PROD2 + #.112 XC
135-Tripropyl Cyclohex. [LP]	2.33e-11	2.33e-11			135PCYC6 + HO. = #.453 RO2-R. + #.545 RO2-N. + #1.106 R2O2. + #.002 RCO-O2. + #.001 CO + #.005 HCHO + #.415 RCHO + #.258 PROD2 + #8.923 XC
135-Tripropyl Cyclohex. [AP]	2.33e-11	2.33e-11			135PCYC6 + HO. = #.453 RO2-R. + #.545 RO2-N. + #1.106 R2O2. + #.002 RCO-O2. + #.001 CO + #.005 HCHO + #.21 RCHO + #8.923 XC + #.258 PRD1 + #.205 PRD2
	3.56e-11	3.56e-11			PRD1 + HO. = #.535 RO2-R. + #.365 RO2-N. + #.575 R2O2. + #.005 CCO-O2. + #.095 RCO-O2. + #.017 HCHO + #.028 CCHO + #.42 RCHO + #.298 PROD2 + #.393 XC
	3.57e-11	3.57e-11			PRD2 + HO. = #.219 RO2-R. + #.178 RO2-N. + #.279 R2O2. + #.603 RCO-O2. + #.03 CO + #.017 HCHO + #.013 CCHO + #.306 RCHO + #.071 PROD2 + #.002 MGLY + #-1.298 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.164 HO2. + #1.276 RO2-R. + #.459 RO2-N. + #.1 RCO-O2. + CO + #.523 RCHO + #.243 PROD2 + #.009 MGLY + #-4.105 XC
1-Methyl-2-Octyl Cyclohex. [LP]	2.22e-11	2.22e-11			1M2C8CC6 + HO. = #.462 RO2-R. + #.538 RO2-N. + #1.035 R2O2. + #.003 HCHO + #.008 CCHO + #.105 RCHO + #.394 PROD2 + #9.08 XC
1-Methyl-2-Octyl Cyclohex. [AP]	2.22e-11	2.22e-11			1M2C8CC6 + HO. = #.462 RO2-R. + #.538 RO2-N. + #1.035 R2O2. + #.003 HCHO + #.008 CCHO + #.105 RCHO + #9.08 XC + #.394 PRD1
	4.19e-11	4.19e-11			PRD1 + HO. = #.214 HO2. + #.529 RO2-R. + #.211 RO2-N. + #.054 R2O2. + #.011 CCO-O2. + #.035 RCO-O2. + #.003 HCHO + #.008 CCHO + #.275 RCHO + #.619 PROD2 + #.052 XC
Nonyl Cyclo-hexane [LP]	2.20e-11	2.20e-11			C9-CYCC6 + HO. = #.509 RO2-R. + #.49 RO2-N. + #.838 R2O2. + #.058 RCHO + #.465 PROD2 + #9.091 XC
Nonyl Cyclo-hexane [AP]	2.20e-11	2.20e-11			C9-CYCC6 + HO. = #.509 RO2-R. + #.49 RO2-N. + #.838 R2O2. + #.058 RCHO + #9.091 XC + #.465 PRD1
	3.09e-11	3.09e-11			PRD1 + HO. = #.038 HO2. + #.57 RO2-R. + #.329 RO2-N. + #.34 R2O2. + #.002 CCO-O2. + #.061 RCO-O2. + #.012 HCHO + #.004 CCHO + #.317 RCHO + #.458 PROD2 + #.118 XC
1,3-Prop.-5-Butyl Cyclohex. [LP]	2.47e-11	2.47e-11			13P5BCC6 + HO. = #.461 RO2-R. + #.538 RO2-N. + #1.045 R2O2. + #.001 RCO-O2. + #.001 CO + #.003 HCHO + #.013 CCHO + #.322 RCHO + #.318 PROD2 + #9.863 XC
1,3-Prop.-5-Butyl Cyclohex. [AP]	2.47e-11	2.47e-11			13P5BCC6 + HO. = #.461 RO2-R. + #.538 RO2-N. + #1.045 R2O2. + #.001 RCO-O2. + #.001 CO + #.003 HCHO + #.013 CCHO + #.126 RCHO + #9.863 XC + #.318 PRD1 + #.196 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b]				Reactions and Products [c]
	k(298)	A	Ea	B	
	2.89e-11	2.89e-11			PRD1 + HO. = #.494 RO2-R. + #.433 RO2-N. + #.754 R2O2. + #.017 CCO-O2. + #.057 RCO-O2. + #.025 HCHO + #.011 CCHO + #.453 RCHO + #.305 PROD2 + #-0.036 XC
	3.24e-11	3.24e-11			PRD2 + HO. = #.182 RO2-R. + #.126 RO2-N. + #.194 R2O2. + #.692 RCO-O2. + #.037 CO + #.014 HCHO + #.016 CCHO + #.227 RCHO + #.046 PROD2 + #.001 MGLY + #-0.877 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.468 HO2. + #1.17 RO2-R. + #.309 RO2-N. + #.053 RCO-O2. + CO + #.645 RCHO + #.165 PROD2 + #.005 MGLY + #-2.95 XC
1-Methyl-4-Nonyl Cyclohex. [LP]	2.36e-11	2.36e-11			1M4C9CY6 + HO. = #.458 RO2-R. + #.541 RO2-N. + #1.018 R2O2. + #.001 HCHO + #.113 RCHO + #.367 PROD2 + #10.209 XC
1-Methyl-4-Nonyl Cyclohex. [AP]	2.36e-11	2.36e-11			1M4C9CY6 + HO. = #.458 RO2-R. + #.541 RO2-N. + #1.018 R2O2. + #.001 HCHO + #10.209 XC + #.367 PRD1 + #.113 PRD2
	3.57e-11	3.57e-11			PRD1 + HO. = #.012 HO2. + #.633 RO2-R. + #.287 RO2-N. + #.15 R2O2. + #.068 RCO-O2. + #.013 HCHO + #.01 CCHO + #.429 RCHO + #.446 PROD2 + #.082 XC
	4.94e-11	4.94e-11			PRD2 + HO. = #.136 HO2. + #.267 RO2-R. + #.149 RO2-N. + #.141 R2O2. + #.017 CCO-O2. + #.431 RCO-O2. + #.001 CO + #.533 RCHO + #.003 PROD2 + #.003 GLY + #.002 MGLY + #-0.853 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.49 HO2. + #1.041 RO2-R. + #.379 RO2-N. + #.091 CCO-O2. + CO + #.352 HCHO + #.143 RCHO + #.499 PROD2 + #-4.227 XC
Decyl Cyclo-hexane [LP]	2.34e-11	2.34e-11			C10CYCC6 + HO. = #.508 RO2-R. + #.492 RO2-N. + #.834 R2O2. + #.055 RCHO + #.467 PROD2 + #10.085 XC
Decyl Cyclo-hexane [AP]	2.34e-11	2.34e-11			C10CYCC6 + HO. = #.508 RO2-R. + #.492 RO2-N. + #.834 R2O2. + #.055 RCHO + #10.085 XC + #.467 PRD1
	3.31e-11	3.31e-11			PRD1 + HO. = #.037 HO2. + #.561 RO2-R. + #.342 RO2-N. + #.376 R2O2. + #.061 RCO-O2. + #.011 HCHO + #.004 CCHO + #.286 RCHO + #.459 PROD2 + #.137 XC
Ethene [LP]	8.52e-12	1.96e-12	-0.87		ETHENE + HO. = RO2-R. + #1.611 HCHO + #.195 CCHO
	1.59e-18	9.14e-15	5.13		ETHENE + O3 = #.12 HO. + #.12 HO2. + #.5 CO + #.13 CO2 + HCHO + #.37 HCOOH
	2.05e-16	4.39e-13	4.54	2.0	ETHENE + NO3 = RO2-R. + RCHO + #-1 XC + XN
	7.29e-13	1.04e-11	1.57		ETHENE + O3P = #.5 HO2. + #.2 RO2-R. + #.3 C-O2. + #.491 CO + #.191 HCHO + #.25 CCHO + #.009 GLY + #.25 INERT + #.25 XC
Ethene [AP]	8.52e-12	1.96e-12	-0.87		ETHENE + HO. = RO2-R. + #1.611 HCHO + #.195 CCHO
	1.59e-18	9.14e-15	5.13		ETHENE + O3 = #.12 HO. + #.12 HO2. + #.5 CO + #.13 CO2 + HCHO + #.37 HCOOH
	2.05e-16	4.39e-13	4.54	2.0	ETHENE + NO3 = RO2-R. + #-1 XC + PRD1 + XN
	7.29e-13	1.04e-11	1.57		ETHENE + O3P = #.5 HO2. + #.2 RO2-R. + #.3 C-O2. + #.491 CO + #.191 HCHO + #.25 CCHO + #.009 GLY + #.25 INERT + #.25 XC
	1.93e-11	1.93e-11			PRD1 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD1 + HV = NO2 + HO2. + CO + HCHO + XC
Propene	2.63e-11	4.85e-12	-1.00		PROPENE + HO. = #.984 RO2-R. + #.016 RO2-N. + #.984 HCHO + #.984 CCHO + #-0.048 XC
	1.01e-17	5.51e-15	3.73		PROPENE + O3 = #.32 HO. + #.06 HO2. + #.26 C-O2. + #.51 CO + #.135 CO2 + #.5 HCHO + #.5 CCHO + #.185 HCOOH + #.17 CCO-OH + #.07 INERT + #.07 XC
	9.49e-15	4.59e-13	2.30		PROPENE + NO3 = #.949 RO2-R. + #.051 RO2-N. + #2.693 XC + XN
	3.98e-12	1.18e-11	0.64		PROPENE + O3P = #.45 RCHO + #.55 MEK + #-0.55 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
1-Butene [LP]	3.14e-11	6.55e-12	-0.93		1-BUTENE + HO. = #.975 RO2-R. + #.025 RO2-N. + #.006 R2O2. + #.969 HCHO + #.975 RCHO + #-0.045 XC
	9.65e-18	3.36e-15	3.47		1-BUTENE + O3 = #.116 HO. + #.06 HO2. + #.057 RO2-R. + #.306 CO + #.065 CO2 + #.5 HCHO + #.057 CCHO + #.5 RCHO + #.185 HCOOH + #.444 RCO-OH
	1.35e-14	3.14e-13	1.86		1-BUTENE + NO3 = #.92 RO2-R. + #.08 RO2-N. + #.075 R2O2. + #.075 CCHO + #.075 RCHO + #.844 RNO3 + #-1.925 XC + #.156 XN
	4.18e-12	1.25e-11	0.65		1-BUTENE + O3P = #.45 RCHO + #.55 MEK + #.45 XC
1-Butene [AP]	3.14e-11	6.55e-12	-0.93		1-BUTENE + HO. = #.975 RO2-R. + #.025 RO2-N. + #.006 R2O2. + #.969 HCHO + #.975 RCHO + #-0.045 XC
	9.65e-18	3.36e-15	3.47		1-BUTENE + O3 = #.116 HO. + #.06 HO2. + #.057 RO2-R. + #.306 CO + #.065 CO2 + #.5 HCHO + #.057 CCHO + #.5 RCHO + #.185 HCOOH + #.444 RCO-OH
	1.35e-14	3.14e-13	1.86		1-BUTENE + NO3 = #.92 RO2-R. + #.08 RO2-N. + #.075 R2O2. + #.075 CCHO + #.844 RNO3 + #-1.925 XC + #.075 PRD1 + #.156 XN
	4.18e-12	1.25e-11	0.65		1-BUTENE + O3P = #.55 MEK + #.45 XC + #.45 PRD2
	1.93e-11	1.93e-11			PRD1 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD1 + HV = NO2 + HO2. + CO + HCHO + XC
	2.33e-11	2.33e-11			PRD2 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
1-Pentene [LP]	3.14e-11	5.86e-12	-0.99		1-PENTEN + HO. = #.927 RO2-R. + #.073 RO2-N. + #.121 R2O2. + #.814 HCHO + #.907 RCHO + #.021 PROD2 + #.906 XC
	1.00e-17	3.36e-15	3.45		1-PENTEN + O3 = #.101 HO. + #.06 HO2. + #.04 RO2-R. + #.001 RO2-N. + #.291 CO + #.065 CO2 + #.5 HCHO + #.54 RCHO + #.185 HCOOH + #.46 RCO-OH + #.955 XC
	1.38e-14	1.38e-14			1-PENTEN + NO3 = #.834 RO2-R. + #.166 RO2-N. + #.781 R2O2. + #.033 RCHO + #.818 RNO3 + #-1.001 XC + #.182 XN
	4.65e-12	1.48e-11	0.69		1-PENTEN + O3P = #.45 RCHO + #.55 MEK + #1.45 XC
1-Pentene [AP]	3.14e-11	5.86e-12	-0.99		1-PENTEN + HO. = #.927 RO2-R. + #.073 RO2-N. + #.121 R2O2. + #.814 HCHO + #.021 PROD2 + #.906 XC + #.907 PRD1
	1.00e-17	3.36e-15	3.45		1-PENTEN + O3 = #.101 HO. + #.06 HO2. + #.04 RO2-R. + #.001 RO2-N. + #.291 CO + #.065 CO2 + #.5 HCHO + #.04 RCHO + #.185 HCOOH + #.46 RCO-OH + #.955 XC + #.5 PRD2
	1.38e-14	1.38e-14			1-PENTEN + NO3 = #.834 RO2-R. + #.166 RO2-N. + #.781 R2O2. + #.033 RCHO + #.818 RNO3 + #-1.001 XC + #.182 XN
	4.65e-12	1.48e-11	0.69		1-PENTEN + O3P = #.55 MEK + #1.45 XC + #.45 PRD3
	2.45e-11	2.45e-11			PRD1 + HO. = #.042 HO2. + #.083 RO2-R. + #.007 RO2-N. + #.013 R2O2. + #.868 RCO-O2. + #.047 CO + #.013 HCHO + #.017 CCHO + #.093 RCHO + #.001 GLY + #.018 MGLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #1.102 HO2. + #.88 RO2-R. + #.018 RO2-N. + CO + #.982 RCHO + #-1.054 XC
	2.33e-11	2.33e-11			PRD2 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	2.82e-11	2.82e-11			PRD3 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC
3-Methyl-1-Butene [LP]	3.18e-11	5.32e-12	-1.06		3M-1-BUT + HO. = #.928 RO2-R. + #.072 RO2-N. + #.174 R2O2. + #.749 HCHO + #.174 CCHO + #.749 RCHO + #.167 ACET + #.012 PROD2 + #.651 XC
	1.10e-17	3.36e-15	3.39		3M-1-BUT + O3 = #.101 HO. + #.06 HO2. + #.039 RO2-R. + #.002 RO2-N. + #.291 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.039 ACET + #.185 HCOOH + #.46 RCO-OH + #.953 XC
	1.38e-14	1.38e-14			3M-1-BUT + NO3 = #.851 RO2-R. + #.149 RO2-N. + #.827 R2O2. + #.827 RCHO + #.794 ACET + #.057 RNO3 + #-1.099 XC + #.943 XN
	4.14e-12	1.32e-11	0.69		3M-1-BUT + O3P = #.45 RCHO + #.55 MEK + #1.45 XC
3-Methyl-1-Butene [AP]	3.18e-11	5.32e-12	-1.06		3M-1-BUT + HO. = #.928 RO2-R. + #.072 RO2-N. + #.174 R2O2. + #.749 HCHO + #.174 CCHO + #.167 ACET + #.012 PROD2 + #.651 XC + #.749 PRD1
	1.10e-17	3.36e-15	3.39		3M-1-BUT + O3 = #.101 HO. + #.06 HO2. + #.039 RO2-R. + #.002 RO2-N. + #.291 CO + #.065 CO2 + #.5 HCHO + #.039 ACET + #.185 HCOOH + #.46 RCO-OH + #.953 XC + #.5 PRD2
	1.38e-14	1.38e-14			3M-1-BUT + NO3 = #.851 RO2-R. + #.149 RO2-N. + #.827 R2O2. + #.794 ACET + #.057 RNO3 + #-1.099 XC + #.827 PRD2 + #.943 XN
	4.14e-12	1.32e-11	0.69		3M-1-BUT + O3P = #.55 MEK + #1.45 XC + #.45 PRD3
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	1.93e-11	1.93e-11			PRD2 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD2 + HV = NO2 + HO2. + CO + HCHO + XC
	2.74e-11	2.74e-11			PRD3 + HO. = #.129 RO2-R. + #.012 RO2-N. + #.112 R2O2. + #.002 C-O2. + #.856 RCO-O2. + #.125 CO + #.092 HCHO + #.036 RCHO + #.096 ACET + #.004 GLY + #-0.264 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.652 HO2. + #1.294 RO2-R. + #.053 RO2-N. + CO + #.348 HCHO + #.613 RCHO + #.334 ACET + #-1.508 XC
1-Hexene [LP]	3.70e-11	6.91e-12	-0.99		1-HEXENE + HO. = #.904 RO2-R. + #.096 RO2-N. + #.419 R2O2. + #.526 HCHO + #.635 RCHO + #.269 PROD2 + #1.38 XC
	1.10e-17	3.36e-15	3.39		1-HEXENE + O3 = #.085 HO. + #.041 HO2. + #.042 RO2-R. + #.002 RO2-N. + #.275 CO + #.065 CO2 + #.5 HCHO + #.523 RCHO + #.475 PROD2 + #.185 HCOOH + #.545 XC
	1.38e-14	1.38e-14			1-HEXENE + NO3 = #.763 RO2-R. + #.237 RO2-N. + #.845 R2O2. + #.763 RNO3 + #.237 XN
	4.65e-12	1.48e-11	0.69		1-HEXENE + O3P = #.45 RCHO + #.55 MEK + #2.45 XC
1-Hexene [AP]	3.70e-11	6.91e-12	-0.99		1-HEXENE + HO. = #.904 RO2-R. + #.096 RO2-N. + #.419 R2O2. + #.526 HCHO + #1.38 XC + #.635 PRD1 + #.269 PRD2
	1.10e-17	3.36e-15	3.39		1-HEXENE + O3 = #.085 HO. + #.041 HO2. + #.042 RO2-R. + #.002 RO2-N. + #.275 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #.545 XC + #.523 PRD3 + #.475 PRD4
	1.38e-14	1.38e-14			1-HEXENE + NO3 = #.763 RO2-R. + #.237 RO2-N. + #.845 R2O2. + #.763 RNO3 + #.237 XN
	4.65e-12	1.48e-11	0.69		1-HEXENE + O3P = #.55 MEK + #2.45 XC + #.45 PRD5
	3.00e-11	3.00e-11			PRD1 + HO. = #.074 HO2. + #.084 RO2-R. + #.016 RO2-N. + #.066 R2O2. + #.826 RCO-O2. + #.035 CO + #.009 HCHO + #.017 CCHO + #.129 RCHO + #.034 MGLY + #-0.145 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.546 HO2. + #1.396 RO2-R. + #.057 RO2-N. + CO + #.943 RCHO + #-1.172 XC
	1.70e-11	1.70e-11			PRD2 + HO. = #.575 HO2. + #.305 RO2-R. + #.033 RO2-N. + #.087 RCO-O2. + #.033 HCHO + #.242 CCHO + #.295 RCHO + #.494 PROD2 + #.146 MGLY + #.741 XC
		PF=KETONE QY = 1.0e-2			PRD2 + HV = HO2. + RCO-O2. + HCHO + #2 XC
	2.82e-11	2.82e-11			PRD3 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD3 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC
	6.76e-12	6.76e-12			PRD4 + HO. = #.926 RO2-R. + #.074 RO2-N. + #.549 R2O2. + #.016 CO2 + #.327 CCHO + #.434 RCHO + #.091 PROD2 + #.07 MGLY + #.111 BACL + #.29 RCO-OH + #1.513 XC
	2.43e-11	2.43e-11			PRD5 + HO. = #.112 RO2-R. + #.04 RO2-N. + #.154 R2O2. + #.848 RCO-O2. + #.014 CO + #.002 HCHO + #.103 RCHO + #.018 MGLY + #-0.166 XC
	3.80e-15	3.80e-15			PRD5 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD5 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.874 RCHO + #-1.377 XC
3,3-Dimethyl-1-Butene [LP]	2.80e-11	5.23e-12	-0.99		33M1-BUT + HO. = #.372 RO2-R. + #.119 RO2-N. + #1.044 R2O2. + #.509 TBU-O. + #.369 HCHO + #.53 CCHO + #.371 RCHO + #.001 ACET + #1.213 XC
	5.20e-18	3.36e-15	3.83		33M1-BUT + O3 = #.085 HO. + #.036 HO2. + #.024 RO2-R. + #.001 RO2-N. + #.024 TBU-O. + #.275 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.185 HCOOH + #.475 RCO-OH + #1.972 XC
	1.38e-14	1.38e-14			33M1-BUT + NO3 = #.188 RO2-N. + #1.658 R2O2. + #.812 TBU-O. + #.845 RCHO + #-0.1 XC + XN
	4.39e-12	4.39e-12			33M1-BUT + O3P = #.45 RCHO + #.55 MEK + #2.45 XC
3,3-Dimethyl-1-Butene [AP]	2.80e-11	5.23e-12	-0.99		33M1-BUT + HO. = #.372 RO2-R. + #.119 RO2-N. + #1.044 R2O2. + #.509 TBU-O. + #.369 HCHO + #.53 CCHO + #.001 ACET + #1.213 XC + #.371 PRD1
	5.20e-18	3.36e-15	3.83		33M1-BUT + O3 = #.085 HO. + #.036 HO2. + #.024 RO2-R. + #.001 RO2-N. + #.024 TBU-O. + #.275 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #.475 RCO-OH + #1.972 XC + #.5 PRD2
	1.38e-14	1.38e-14			33M1-BUT + NO3 = #.188 RO2-N. + #1.658 R2O2. + #.812 TBU-O. + #-0.1 XC + #.845 PRD3 + XN
	4.39e-12	4.39e-12			33M1-BUT + O3P = #.55 MEK + #2.45 XC + #.45 PRD4
	2.63e-11	2.63e-11			PRD1 + HO. = #.023 RO2-R. + #.003 RO2-N. + #.024 R2O2. + #.974 RCO-O2. + #.023 CO + #.024 HCHO + #.001 RCHO + #.023 ACET + #-0.054 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 TBU-O. + CO + #-1.118 XC
	2.63e-11	2.63e-11			PRD2 + HO. = #.023 RO2-R. + #.003 RO2-N. + #.024 R2O2. + #.974 RCO-O2. + #.023 CO + #.024 HCHO + #.001 RCHO + #.023 ACET + #-0.054 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 TBU-O. + CO + #-1.118 XC
	1.93e-11	1.93e-11			PRD3 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD3 + HV = NO2 + HO2. + CO + HCHO + XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.06e-11	2.06e-11			PRD4 + HO. = #.039 RO2-R. + #.01 RO2-N. + #.043 R2O2. + #.945 RCO-O2. + #.005 TBU-O. + #.039 CO + #.019 HCHO + #.03 RCHO + #.009 ACET + #.006 GLY + #-0.099 XC
	3.80e-15	3.80e-15			PRD4 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD4 + HV = #1.021 RO2-R. + #.088 RO2-N. + #.819 R2O2. + #.891 TBU-O. + CO + #.928 HCHO + #.021 RCHO + #-2.191 XC
3-Methyl-1-Pentene [LP]	3.16e-11	3.16e-11			3M1-C5E + HO. = #.89 RO2-R. + #.11 RO2-N. + #.178 R2O2. + #.761 HCHO + #.161 CCHO + #.785 RCHO + #.045 MEK + #.023 PROD2 + #1.581 XC
	4.90e-18	3.36e-15	3.87		3M1-C5E + O3 = #.085 HO. + #.051 HO2. + #.032 RO2-R. + #.002 RO2-N. + #.275 CO + #.065 CO2 + #.5 HCHO + #.018 CCHO + #.5 RCHO + #.014 MEK + #.475 PROD2 + #.185 HCOOH + #.521 XC
	1.38e-14	1.38e-14			3M1-C5E + NO3 = #.776 RO2-R. + #.224 RO2-N. + #1.049 R2O2. + #.454 CCHO + #.626 RCHO + #.348 MEK + #.201 RNO3 + #-0.726 XC + #.799 XN
	5.60e-12	5.60e-12			3M1-C5E + O3P = #.45 RCHO + #.55 PROD2 + #1.35 XC
3-Methyl-1-Pentene [AP]	3.16e-11	3.16e-11			3M1-C5E + HO. = #.89 RO2-R. + #.11 RO2-N. + #.178 R2O2. + #.761 HCHO + #.161 CCHO + #.045 MEK + #.023 PROD2 + #1.581 XC + #.785 PRD1
	4.90e-18	3.36e-15	3.87		3M1-C5E + O3 = #.085 HO. + #.051 HO2. + #.032 RO2-R. + #.002 RO2-N. + #.275 CO + #.065 CO2 + #.5 HCHO + #.018 CCHO + #.014 MEK + #.185 HCOOH + #.521 XC + #.5 PRD2 + #.475 PRD3
	1.38e-14	1.38e-14			3M1-C5E + NO3 = #.776 RO2-R. + #.224 RO2-N. + #1.049 R2O2. + #.454 CCHO + #.348 MEK + #.201 RNO3 + #-0.726 XC + #.626 PRD4 + #.799 XN
	5.60e-12	5.60e-12			3M1-C5E + O3P = #1.35 XC + #.55 PRD5 + #.45 PRD6
	2.25e-11	2.25e-11			PRD1 + HO. = #.119 RO2-R. + #.014 RO2-N. + #.046 R2O2. + #.867 RCO-O2. + #.119 CO + #.09 CCHO + #.076 MEK + #-0.284 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.637 HO2. + #1.282 RO2-R. + #.08 RO2-N. + CO + #.725 CCHO + #.557 MEK + #-2.161 XC
	2.25e-11	2.25e-11			PRD2 + HO. = #.119 RO2-R. + #.014 RO2-N. + #.046 R2O2. + #.867 RCO-O2. + #.119 CO + #.09 CCHO + #.076 MEK + #-0.284 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.637 HO2. + #1.282 RO2-R. + #.08 RO2-N. + CO + #.725 CCHO + #.557 MEK + #-2.161 XC
	6.22e-12	6.22e-12			PRD3 + HO. = #.93 RO2-R. + #.07 RO2-N. + #.651 R2O2. + #.342 CO2 + #.026 HCHO + #.635 CCHO + #.08 RCHO + #.265 MEK + #.513 BACL + #.589 XC
	1.93e-11	1.93e-11			PRD4 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD4 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD4 + HV = NO2 + HO2. + CO + HCHO + XC
	5.10e-12	5.10e-12			PRD5 + HO. = #.756 RO2-R. + #.164 RO2-N. + #1.889 R2O2. + #.081 RCO-O2. + #.255 CO + #.043 CO2 + #.056 HCHO + #.173 CCHO + #.024 RCHO + #.57 MEK + #.076 PROD2 + #.299 HCOOH + #.609 XC
	2.45e-11	2.45e-11			PRD6 + HO. = #.158 RO2-R. + #.027 RO2-N. + #.158 R2O2. + #.815 RCO-O2. + #.065 CO + #.038 HCHO + #.101 CCHO + #.115 RCHO + #.034 MEK + #.002 GLY + #.003 MGLY + #-0.406 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.144 HO2. + #1.737 RO2-R. + #.119 RO2-N. + CO + #.138 HCHO + #.1 CCHO + #.754 RCHO + #.077 MEK + #-1.623 XC
4-Methyl-1-Pentene [LP]	3.16e-11	3.16e-11			4M1-C5E + HO. = #.884 RO2-R. + #.116 RO2-N. + #.189 R2O2. + #.717 HCHO + #.001 CCHO + #.846 RCHO + #.001 ACET + #.037 PROD2 + #1.822 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	9.20e-18	3.36e-15	3.49		4M1-C5E + O3 = #.085 HO. + #.051 HO2. + #.032 RO2-R. + #.001 RO2-N. + #.275 CO + #.065 CO2 + #.509 HCHO + #.515 RCHO + #.008 ACET + #.475 PROD2 + #.185 HCOOH + #.537 XC
	1.38e-14	1.38e-14			4M1-C5E + NO3 = #.769 RO2-R. + #.231 RO2-N. + #.8 R2O2. + #.006 HCHO + #.029 RCHO + #.006 ACET + #.752 RNO3 + #-0.009 XC + #.248 XN
	5.60e-12	5.60e-12			4M1-C5E + O3P = #.45 RCHO + #.55 MEK + #2.45 XC
4-Methyl-1-Pentene [AP]	3.16e-11	3.16e-11			4M1-C5E + HO. = #.884 RO2-R. + #.116 RO2-N. + #.189 R2O2. + #.717 HCHO + #.001 CCHO + #.001 ACET + #1.822 XC + #.846 PRD1 + #.037 PRD2
	9.20e-18	3.36e-15	3.49		4M1-C5E + O3 = #.085 HO. + #.051 HO2. + #.032 RO2-R. + #.001 RO2-N. + #.275 CO + #.065 CO2 + #.509 HCHO + #.008 ACET + #.185 HCOOH + #.537 XC + #.515 PRD3 + #.475 PRD4
	1.38e-14	1.38e-14			4M1-C5E + NO3 = #.769 RO2-R. + #.231 RO2-N. + #.8 R2O2. + #.006 HCHO + #.029 RCHO + #.006 ACET + #.752 RNO3 + #-0.009 XC + #.248 XN
	5.60e-12	5.60e-12			4M1-C5E + O3P = #.55 MEK + #2.45 XC + #.45 PRD5
	2.74e-11	2.74e-11			PRD1 + HO. = #.035 HO2. + #.119 RO2-R. + #.011 RO2-N. + #.095 R2O2. + #.002 C-O2. + #.833 RCO-O2. + #.106 CO + #.078 HCHO + #.039 RCHO + #.088 ACET + #.003 GLY + #.036 MGLY + #-0.249 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.86 HO2. + #1.095 RO2-R. + #.045 RO2-N. + CO + #.294 HCHO + #.673 RCHO + #.282 ACET + #-1.429 XC
	1.74e-11	1.74e-11			PRD2 + HO. = #.329 HO2. + #.535 RO2-R. + #.057 RO2-N. + #.078 RCO-O2. + #.522 HCHO + #.001 CCHO + #.28 RCHO + #.484 MEK + #.145 MGLY + #1.682 XC
		PF=KETONE QY = 1.0e-2			PRD2 + HV = HO2. + RCO-O2. + HCHO + #2 XC
	2.74e-11	2.74e-11			PRD3 + HO. = #.129 RO2-R. + #.012 RO2-N. + #.112 R2O2. + #.002 C-O2. + #.856 RCO-O2. + #.125 CO + #.092 HCHO + #.036 RCHO + #.096 ACET + #.004 GLY + #-0.264 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.652 HO2. + #1.294 RO2-R. + #.053 RO2-N. + CO + #.348 HCHO + #.613 RCHO + #.334 ACET + #-1.508 XC
	8.81e-12	8.81e-12			PRD4 + HO. = #.897 RO2-R. + #.067 RO2-N. + #.85 R2O2. + #.036 C-O2. + #.019 CO2 + #.033 HCHO + #.005 CCHO + #.022 RCHO + #.78 ACET + #.781 MGLY + #.068 BACL + #.059 RCO-OH + #.306 XC
	2.42e-11	2.42e-11			PRD5 + HO. = #.092 RO2-R. + #.029 RO2-N. + #.155 R2O2. + #.879 RCO-O2. + #.027 CO + #.09 RCHO + #.051 ACET + #.004 MGLY + #-0.272 XC
	3.80e-15	3.80e-15			PRD5 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD5 + HV = #.159 HO2. + #1.722 RO2-R. + #.119 RO2-N. + CO + #.881 RCHO + #-1.358 XC
1-Heptene [LP]	4.00e-11	7.47e-12	-0.99		1-HEPTEN + HO. = #.807 RO2-R. + #.193 RO2-N. + #.426 R2O2. + #.439 HCHO + #.536 RCHO + #.271 PROD2 + #2.169 XC
	1.20e-17	3.36e-15	3.34		1-HEPTEN + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #1.5 XC
	1.38e-14	1.38e-14			1-HEPTEN + NO3 = #.7 RO2-R. + #.3 RO2-N. + #.809 R2O2. + #.7 RNO3 + XC + #.3 XN
	8.53e-12	8.53e-12			1-HEPTEN + O3P = #.45 RCHO + #.55 PROD2 + #2.35 XC
1-Heptene [AP]	4.00e-11	7.47e-12	-0.99		1-HEPTEN + HO. = #.807 RO2-R. + #.193 RO2-N. + #.426 R2O2. + #.439 HCHO + #2.169 XC + #.536 PRD1 + #.271 PRD2
	1.20e-17	3.36e-15	3.34		1-HEPTEN + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #1.5 XC + #.5 PRD3 + #.5 PRD4

Table A-6 (continued)

Compound [a]	Rate Parameters [b]				Reactions and Products [c]
	k(298)	A	Ea	B	
	1.38e-14	1.38e-14			1-HEPTEN + NO3 = #.7 RO2-R. + #.3 RO2-N. + #.809 R2O2. + #.7 RNO3 + XC + #.3 XN
	8.53e-12	8.53e-12			1-HEPTEN + O3P = #2.35 XC + #.55 PRD5 + #.45 PRD6
	2.71e-11	2.71e-11			PRD1 + HO. = #.07 HO2. + #.111 RO2-R. + #.036 RO2-N. + #.126 R2O2. + #.782 RCO-O2. + #.011 CO + #.002 HCHO + #.151 RCHO + #.048 MGLY + #-0.175 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.414 HO2. + #1.483 RO2-R. + #.103 RO2-N. + CO + #.897 RCHO + #-1.309 XC
	2.00e-11	2.00e-11			PRD2 + HO. = #.555 HO2. + #.308 RO2-R. + #.048 RO2-N. + #.089 RCO-O2. + #.028 HCHO + #.025 CCHO + #.479 RCHO + #.517 PROD2 + #.125 MGLY + #.455 XC
	2.43e-11	2.43e-11			PRD3 + HO. = #.112 RO2-R. + #.04 RO2-N. + #.154 R2O2. + #.848 RCO-O2. + #.014 CO + #.002 HCHO + #.103 RCHO + #.018 MGLY + #-0.166 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.874 RCHO + #-1.377 XC
	8.18e-12	8.18e-12			PRD4 + HO. = #.845 RO2-R. + #.155 RO2-N. + #.766 R2O2. + #.013 CO2 + #.014 CCHO + #.38 RCHO + #.544 PROD2 + #.012 MGLY + #.085 BACL + #.251 XC
	6.26e-12	6.26e-12			PRD5 + HO. = #.686 RO2-R. + #.303 RO2-N. + #1.739 R2O2. + #.011 RCO-O2. + #.175 CO + #.017 CO2 + #.017 HCHO + #.001 CCHO + #.279 RCHO + #.033 MEK + #.383 PROD2 + #.007 BACL + #.109 HCOOH + #.405 XC
	2.57e-11	2.57e-11			PRD6 + HO. = #.136 RO2-R. + #.067 RO2-N. + #.191 R2O2. + #.797 RCO-O2. + #.009 CO + #.118 RCHO + #.017 MGLY + #-0.21 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.814 RCHO + #-1.557 XC
1-Octene [LP]	3.16e-11	3.16e-11			1-OCTENE + HO. = #.754 RO2-R. + #.246 RO2-N. + #.418 R2O2. + #.42 HCHO + #.497 RCHO + #.257 PROD2 + #3.07 XC
	1.40e-17	3.36e-15	3.25		1-OCTENE + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #2.5 XC
	1.38e-14	1.38e-14			1-OCTENE + NO3 = #.645 RO2-R. + #.355 RO2-N. + #.781 R2O2. + #.645 RNO3 + #2 XC + #.355 XN
	5.60e-12	5.60e-12			1-OCTENE + O3P = #.45 RCHO + #.55 PROD2 + #3.35 XC
1-Octene [AP]	3.16e-11	3.16e-11			1-OCTENE + HO. = #.754 RO2-R. + #.246 RO2-N. + #.418 R2O2. + #.42 HCHO + #3.07 XC + #.497 PRD1 + #.257 PRD2
	1.40e-17	3.36e-15	3.25		1-OCTENE + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #2.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-OCTENE + NO3 = #.645 RO2-R. + #.355 RO2-N. + #.781 R2O2. + #.645 RNO3 + #2 XC + #.355 XN
	5.60e-12	5.60e-12			1-OCTENE + O3P = #3.35 XC + #.55 PRD5 + #.45 PRD6
	2.81e-11	2.81e-11			PRD1 + HO. = #.057 HO2. + #.135 RO2-R. + #.061 RO2-N. + #.162 R2O2. + #.747 RCO-O2. + #.007 CO + #.159 RCHO + #.042 MGLY + #-0.215 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.391 HO2. + #1.452 RO2-R. + #.157 RO2-N. + CO + #.843 RCHO + #-1.471 XC
	2.14e-11	2.14e-11			PRD2 + HO. = #.472 HO2. + #.369 RO2-R. + #.077 RO2-N. + #.082 RCO-O2. + #.026 HCHO + #.538 RCHO + #.483 PROD2 + #.116 MGLY + #.401 XC
	2.57e-11	2.57e-11			PRD3 + HO. = #.136 RO2-R. + #.067 RO2-N. + #.191 R2O2. + #.797 RCO-O2. + #.009 CO + #.118 RCHO + #.017 MGLY + #-0.21 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD3 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.814 RCHO + #-1.557 XC
	9.60e-12	9.60e-12			PRD4 + HO. = #.754 RO2-R. + #.246 RO2-N. + #.847 R2O2. + #.011 CO2 + #.058 RCHO + #.647 PROD2 + #.067 BACL + #.189 XC
	7.68e-12	7.68e-12			PRD5 + HO. = #.599 RO2-R. + #.391 RO2-N. + #1.629 R2O2. + #.009 RCO-O2. + #.133 CO + #.013 CO2 + #.013 HCHO + #.198 RCHO + #.404 PROD2 + #.005 BACL + #.084 HCOOH + #.251 XC
	2.71e-11	2.71e-11			PRD6 + HO. = #.164 RO2-R. + #.096 RO2-N. + #.219 R2O2. + #.74 RCO-O2. + #.008 CO + #.149 RCHO + #.015 MGLY + #-0.296 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.135 HO2. + #1.613 RO2-R. + #.252 RO2-N. + CO + #.748 RCHO + #-1.756 XC
1-Nonene [LP]	3.16e-11	3.16e-11			1-C9E + HO. = #.708 RO2-R. + #.292 RO2-N. + #.417 R2O2. + #.403 HCHO + #.471 RCHO + #.237 PROD2 + #4.009 XC
	1.01e-17	1.01e-17			1-C9E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #3.5 XC
	1.38e-14	1.38e-14			1-C9E + NO3 = #.597 RO2-R. + #.403 RO2-N. + #.794 R2O2. + #.597 RNO3 + #3 XC + #.403 XN
	5.60e-12	5.60e-12			1-C9E + O3P = #.45 RCHO + #.55 PROD2 + #4.35 XC
1-Nonene [AP]	3.16e-11	3.16e-11			1-C9E + HO. = #.708 RO2-R. + #.292 RO2-N. + #.417 R2O2. + #.403 HCHO + #4.009 XC + #.471 PRD1 + #.237 PRD2
	1.01e-17	1.01e-17			1-C9E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #3.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C9E + NO3 = #.597 RO2-R. + #.403 RO2-N. + #.794 R2O2. + #.597 RNO3 + #3 XC + #.403 XN
	5.60e-12	5.60e-12			1-C9E + O3P = #4.35 XC + #.55 PRD5 + #.45 PRD6
	2.94e-11	2.94e-11			PRD1 + HO. = #.048 HO2. + #.164 RO2-R. + #.089 RO2-N. + #.187 R2O2. + #.699 RCO-O2. + #.007 CO + #.181 RCHO + #.038 MGLY + #-0.294 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.402 HO2. + #1.382 RO2-R. + #.216 RO2-N. + CO + #.784 RCHO + #-1.648 XC
	2.29e-11	2.29e-11			PRD2 + HO. = #.433 HO2. + #.39 RO2-R. + #.101 RO2-N. + #.075 RCO-O2. + #.024 HCHO + #.489 RCHO + #.495 PROD2 + #.109 MGLY + #.376 XC
	2.71e-11	2.71e-11			PRD3 + HO. = #.164 RO2-R. + #.096 RO2-N. + #.219 R2O2. + #.74 RCO-O2. + #.008 CO + #.149 RCHO + #.015 MGLY + #-0.296 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.135 HO2. + #1.613 RO2-R. + #.252 RO2-N. + CO + #.748 RCHO + #-1.756 XC
	1.10e-11	1.10e-11			PRD4 + HO. = #.683 RO2-R. + #.317 RO2-N. + #.826 R2O2. + #.01 RCHO + #.62 PROD2 + #.054 BACL + #.137 XC
	9.10e-12	9.10e-12			PRD5 + HO. = #.532 RO2-R. + #.461 RO2-N. + #1.534 R2O2. + #.007 RCO-O2. + #.117 CO + #.01 CO2 + #.01 HCHO + #.165 RCHO + #.367 PROD2 + #.004 BACL + #.067 HCOOH + #.217 XC
	2.85e-11	2.85e-11			PRD6 + HO. = #.178 RO2-R. + #.123 RO2-N. + #.243 R2O2. + #.699 RCO-O2. + #.007 CO + #.166 RCHO + #.012 MGLY + #-0.375 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.082 HO2. + #1.585 RO2-R. + #.333 RO2-N. + CO + #.592 RCHO + #.076 PROD2 + #-2.225 XC
1-Decene [LP]	3.16e-11	3.16e-11			1-C10E + HO. = #.676 RO2-R. + #.324 RO2-N. + #.408 R2O2. + #.391 HCHO + #.455 RCHO + #.222 PROD2 + #4.973 XC
	9.30e-18	3.36e-15	3.49		1-C10E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #4.5 XC
	1.38e-14	1.38e-14			1-C10E + NO3 = #.567 RO2-R. + #.433 RO2-N. + #.791 R2O2. + #.567 RNO3 + #4 XC + #.433 XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	5.60e-12	5.60e-12			1-C10E + O3P = #.45 RCHO + #.55 PROD2 + #5.35 XC
1-Decene [AP]	3.16e-11	3.16e-11			1-C10E + HO. = #.676 RO2-R. + #.324 RO2-N. + #.408 R2O2. + #.391 HCHO + #4.973 XC + #.455 PRD1 + #.222 PRD2
	9.30e-18	3.36e-15	3.49		1-C10E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #4.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C10E + NO3 = #.567 RO2-R. + #.433 RO2-N. + #.791 R2O2. + #.567 RNO3 + #4 XC + #.433 XN
	5.60e-12	5.60e-12			1-C10E + O3P = #5.35 XC + #.55 PRD5 + #.45 PRD6
	3.07e-11	3.07e-11			PRD1 + HO. = #.042 HO2. + #.182 RO2-R. + #.114 RO2-N. + #.21 R2O2. + #.663 RCO-O2. + #.006 CO + #.195 RCHO + #.034 MGLY + #-0.364 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.349 HO2. + #1.364 RO2-R. + #.286 RO2-N. + CO + #.649 RCHO + #.065 PROD2 + #-2.054 XC
	2.43e-11	2.43e-11			PRD2 + HO. = #.371 HO2. + #.437 RO2-R. + #.131 RO2-N. + #.062 RCO-O2. + #.023 HCHO + #.421 RCHO + #.514 PROD2 + #.103 MGLY + #.354 XC
	2.85e-11	2.85e-11			PRD3 + HO. = #.178 RO2-R. + #.123 RO2-N. + #.243 R2O2. + #.699 RCO-O2. + #.007 CO + #.166 RCHO + #.012 MGLY + #-0.375 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.082 HO2. + #1.585 RO2-R. + #.333 RO2-N. + CO + #.592 RCHO + #.076 PROD2 + #-2.225 XC
	1.24e-11	1.24e-11			PRD4 + HO. = #.627 RO2-R. + #.373 RO2-N. + #.806 R2O2. + #.004 RCHO + #.584 PROD2 + #.039 BACL + #.09 XC
	1.05e-11	1.05e-11			PRD5 + HO. = #.501 RO2-R. + #.493 RO2-N. + #1.371 R2O2. + #.006 RCO-O2. + #.092 CO + #.008 CO2 + #.008 HCHO + #.126 RCHO + #.376 PROD2 + #.002 BACL + #.051 HCOOH + #.162 XC
	2.99e-11	2.99e-11			PRD6 + HO. = #.189 RO2-R. + #.146 RO2-N. + #.268 R2O2. + #.665 RCO-O2. + #.006 CO + #.178 RCHO + #.011 MGLY + #-0.444 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.097 HO2. + #1.51 RO2-R. + #.393 RO2-N. + CO + #.521 RCHO + #.087 PROD2 + #-2.438 XC
1-Undecene [LP]	3.16e-11	3.16e-11			1-C11E + HO. = #.657 RO2-R. + #.343 RO2-N. + #.399 R2O2. + #.383 HCHO + #.444 RCHO + #.212 PROD2 + #5.949 XC
	1.01e-17	1.01e-17			1-C11E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #5.5 XC
	1.38e-14	1.38e-14			1-C11E + NO3 = #.55 RO2-R. + #.45 RO2-N. + #.782 R2O2. + #.55 RNO3 + #5 XC + #.45 XN
	5.60e-12	5.60e-12			1-C11E + O3P = #.45 RCHO + #.55 PROD2 + #6.35 XC
1-Undecene [AP]	3.16e-11	3.16e-11			1-C11E + HO. = #.657 RO2-R. + #.343 RO2-N. + #.399 R2O2. + #.383 HCHO + #5.949 XC + #.444 PRD1 + #.212 PRD2
	1.01e-17	1.01e-17			1-C11E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #5.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C11E + NO3 = #.55 RO2-R. + #.45 RO2-N. + #.782 R2O2. + #.55 RNO3 + #5 XC + #.45 XN
	5.60e-12	5.60e-12			1-C11E + O3P = #6.35 XC + #.55 PRD5 + #.45 PRD6
	3.21e-11	3.21e-11			PRD1 + HO. = #.036 HO2. + #.195 RO2-R. + #.136 RO2-N. + #.231 R2O2. + #.632 RCO-O2. + #.005 CO + #.205 RCHO + #.031 MGLY + #-0.429 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.358 HO2. + #1.303 RO2-R. + #.339 RO2-N. + CO + #.586 RCHO + #.075 PROD2 + #-2.241 XC
	2.57e-11	2.57e-11			PRD2 + HO. = #.301 HO2. + #.485 RO2-R. + #.158 RO2-N. + #.056 RCO-O2. + #.022 HCHO + #.391 RCHO + #.511 PROD2 + #.097 MGLY + #.334 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.99e-11	2.99e-11			PRD3 + HO. = #.189 RO2-R. + #.146 RO2-N. + #.268 R2O2. + #.665 RCO-O2. + #.006 CO + #.178 RCHO + #.011 MGLY + #-0.444 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.097 HO2. + #1.51 RO2-R. + #.393 RO2-N. + CO + #.521 RCHO + #.087 PROD2 + #-2.438 XC
	1.39e-11	1.39e-11			PRD4 + HO. = #.586 RO2-R. + #.414 RO2-N. + #.799 R2O2. + #.006 RCHO + #.548 PROD2 + #.032 BACL + #.082 XC
	1.19e-11	1.19e-11			PRD5 + HO. = #.496 RO2-R. + #.5 RO2-N. + #1.228 R2O2. + #.004 RCO-O2. + #.077 CO + #.007 CO2 + #.007 HCHO + #.105 RCHO + #.391 PROD2 + #.002 BACL + #.043 HCOOH + #.136 XC
	3.14e-11	3.14e-11			PRD6 + HO. = #.2 RO2-R. + #.166 RO2-N. + #.289 R2O2. + #.634 RCO-O2. + #.006 CO + #.19 RCHO + #.01 MGLY + #-0.503 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.127 HO2. + #1.442 RO2-R. + #.431 RO2-N. + CO + #.49 RCHO + #.079 PROD2 + #-2.53 XC
1-Dodecene [LP]	3.16e-11	3.16e-11			1-C12E + HO. = #.644 RO2-R. + #.356 RO2-N. + #.395 R2O2. + #.379 HCHO + #.438 RCHO + #.207 PROD2 + #6.935 XC
	1.01e-17	1.01e-17			1-C12E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #6.5 XC
	1.38e-14	1.38e-14			1-C12E + NO3 = #.539 RO2-R. + #.461 RO2-N. + #.778 R2O2. + #.539 RNO3 + #6 XC + #.461 XN
	5.60e-12	5.60e-12			1-C12E + O3P = #.45 RCHO + #.55 PROD2 + #7.35 XC
1-Dodecene [AP]	3.16e-11	3.16e-11			1-C12E + HO. = #.644 RO2-R. + #.356 RO2-N. + #.395 R2O2. + #.379 HCHO + #6.935 XC + #.438 PRD1 + #.207 PRD2
	1.01e-17	1.01e-17			1-C12E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #6.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C12E + NO3 = #.539 RO2-R. + #.461 RO2-N. + #.778 R2O2. + #.539 RNO3 + #6 XC + #.461 XN
	5.60e-12	5.60e-12			1-C12E + O3P = #7.35 XC + #.55 PRD5 + #.45 PRD6
	3.35e-11	3.35e-11			PRD1 + HO. = #.032 HO2. + #.209 RO2-R. + #.155 RO2-N. + #.25 R2O2. + #.604 RCO-O2. + #.005 CO + #.216 RCHO + #.029 MGLY + #-0.485 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.381 HO2. + #1.246 RO2-R. + #.372 RO2-N. + CO + #.559 RCHO + #.068 PROD2 + #-2.323 XC
	2.71e-11	2.71e-11			PRD2 + HO. = #.246 HO2. + #.522 RO2-R. + #.179 RO2-N. + #.053 RCO-O2. + #.021 HCHO + #.362 RCHO + #.512 PROD2 + #.092 MGLY + #.316 XC
	3.14e-11	3.14e-11			PRD3 + HO. = #.2 RO2-R. + #.166 RO2-N. + #.289 R2O2. + #.634 RCO-O2. + #.006 CO + #.19 RCHO + #.01 MGLY + #-0.503 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.127 HO2. + #1.442 RO2-R. + #.431 RO2-N. + CO + #.49 RCHO + #.079 PROD2 + #-2.53 XC
	1.53e-11	1.53e-11			PRD4 + HO. = #.561 RO2-R. + #.439 RO2-N. + #.788 R2O2. + #.005 RCHO + #.528 PROD2 + #.028 BACL + #.071 XC
	1.34e-11	1.34e-11			PRD5 + HO. = #.498 RO2-R. + #.499 RO2-N. + #1.126 R2O2. + #.003 RCO-O2. + #.063 CO + #.006 CO2 + #.006 HCHO + #.092 RCHO + #.406 PROD2 + #.001 BACL + #.037 HCOOH + #.123 XC
	3.28e-11	3.28e-11			PRD6 + HO. = #.211 RO2-R. + #.182 RO2-N. + #.309 R2O2. + #.606 RCO-O2. + #.006 CO + #.202 RCHO + #.009 MGLY + #-0.553 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.143 HO2. + #1.402 RO2-R. + #.456 RO2-N. + CO + #.471 RCHO + #.074 PROD2 + #-2.588 XC
1-Tridecene [LP]	3.16e-11	3.16e-11			1-C13E + HO. = #.637 RO2-R. + #.363 RO2-N. + #.392 R2O2. + #.376 HCHO + #.434 RCHO + #.203 PROD2 + #7.926 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.01e-17	1.01e-17			1-C13E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #7.5 XC
	1.38e-14	1.38e-14			1-C13E + NO3 = #.532 RO2-R. + #.468 RO2-N. + #.775 R2O2. + #.532 RNO3 + #7 XC + #.468 XN
	5.60e-12	5.60e-12			1-C13E + O3P = #.45 RCHO + #.55 PROD2 + #8.35 XC
1-Tridecene [AP]	3.16e-11	3.16e-11			1-C13E + HO. = #.637 RO2-R. + #.363 RO2-N. + #.392 R2O2. + #.376 HCHO + #7.926 XC + #.434 PRD1 + #.203 PRD2
	1.01e-17	1.01e-17			1-C13E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #7.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C13E + NO3 = #.532 RO2-R. + #.468 RO2-N. + #.775 R2O2. + #.532 RNO3 + #7 XC + #.468 XN
	5.60e-12	5.60e-12			1-C13E + O3P = #8.35 XC + #.55 PRD5 + #.45 PRD6
	3.49e-11	3.49e-11			PRD1 + HO. = #.028 HO2. + #.222 RO2-R. + #.172 RO2-N. + #.267 R2O2. + #.578 RCO-O2. + #.005 CO + #.226 RCHO + #.028 MGLY + #-0.533 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.393 HO2. + #1.213 RO2-R. + #.394 RO2-N. + CO + #.542 RCHO + #.064 PROD2 + #-2.374 XC
	2.85e-11	2.85e-11			PRD2 + HO. = #.195 HO2. + #.558 RO2-R. + #.197 RO2-N. + #.05 RCO-O2. + #.02 HCHO + #.339 RCHO + #.512 PROD2 + #.087 MGLY + #.3 XC
	3.28e-11	3.28e-11			PRD3 + HO. = #.211 RO2-R. + #.182 RO2-N. + #.309 R2O2. + #.606 RCO-O2. + #.006 CO + #.202 RCHO + #.009 MGLY + #-0.553 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.143 HO2. + #1.402 RO2-R. + #.456 RO2-N. + CO + #.471 RCHO + #.074 PROD2 + #-2.588 XC
	1.67e-11	1.67e-11			PRD4 + HO. = #.546 RO2-R. + #.454 RO2-N. + #.78 R2O2. + #.005 RCHO + #.517 PROD2 + #.025 BACL + #.063 XC
	1.48e-11	1.48e-11			PRD5 + HO. = #.495 RO2-R. + #.502 RO2-N. + #1.075 R2O2. + #.003 RCO-O2. + #.056 CO + #.005 CO2 + #.005 HCHO + #.082 RCHO + #.414 PROD2 + #.001 BACL + #.033 HCOOH + #.11 XC
	3.42e-11	3.42e-11			PRD6 + HO. = #.222 RO2-R. + #.197 RO2-N. + #.327 R2O2. + #.581 RCO-O2. + #.005 CO + #.214 RCHO + #.009 MGLY + #-0.596 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.153 HO2. + #1.376 RO2-R. + #.471 RO2-N. + CO + #.459 RCHO + #.07 PROD2 + #-2.623 XC
1-Tetradecene [LP]	3.16e-11	3.16e-11			1-C14E + HO. = #.632 RO2-R. + #.368 RO2-N. + #.39 R2O2. + #.374 HCHO + #.432 RCHO + #.201 PROD2 + #8.921 XC
	1.01e-17	1.01e-17			1-C14E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #8.5 XC
	1.38e-14	1.38e-14			1-C14E + NO3 = #.528 RO2-R. + #.472 RO2-N. + #.773 R2O2. + #.528 RNO3 + #8 XC + #.472 XN
	5.60e-12	5.60e-12			1-C14E + O3P = #.45 RCHO + #.55 PROD2 + #9.35 XC
1-Tetradecene [AP]	3.16e-11	3.16e-11			1-C14E + HO. = #.632 RO2-R. + #.368 RO2-N. + #.39 R2O2. + #.374 HCHO + #8.921 XC + #.432 PRD1 + #.201 PRD2
	1.01e-17	1.01e-17			1-C14E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #8.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C14E + NO3 = #.528 RO2-R. + #.472 RO2-N. + #.773 R2O2. + #.528 RNO3 + #8 XC + #.472 XN
	5.60e-12	5.60e-12			1-C14E + O3P = #9.35 XC + #.55 PRD5 + #.45 PRD6
	3.63e-11	3.63e-11			PRD1 + HO. = #.024 HO2. + #.235 RO2-R. + #.186 RO2-N. + #.283 R2O2. + #.555 RCO-O2. + #.005 CO + #.236 RCHO + #.027 MGLY + #-0.574 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.401 HO2. + #1.191 RO2-R. + #.408 RO2-N. + CO + #.531 RCHO + #.061 PROD2 + #-2.406 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.00e-11	3.00e-11			PRD2 + HO. = #.152 HO2. + #.589 RO2-R. + #.212 RO2-N. + #.047 RCO-O2. + #.019 HCHO + #.317 RCHO + #.514 PROD2 + #.083 MGLY + #.286 XC
	3.42e-11	3.42e-11			PRD3 + HO. = #.222 RO2-R. + #.197 RO2-N. + #.327 R2O2. + #.581 RCO-O2. + #.005 CO + #.214 RCHO + #.009 MGLY + #-0.596 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.153 HO2. + #1.376 RO2-R. + #.471 RO2-N. + CO + #.459 RCHO + #.07 PROD2 + #-2.623 XC
	1.81e-11	1.81e-11			PRD4 + HO. = #.539 RO2-R. + #.461 RO2-N. + #.769 R2O2. + #.516 PROD2 + #.023 BACL + #.045 XC
	1.62e-11	1.62e-11			PRD5 + HO. = #.493 RO2-R. + #.504 RO2-N. + #1.04 R2O2. + #.003 RCO-O2. + #.05 CO + #.005 CO2 + #.005 HCHO + #.074 RCHO + #.42 PROD2 + #.001 BACL + #.03 HCOOH + #.1 XC
	3.56e-11	3.56e-11			PRD6 + HO. = #.233 RO2-R. + #.21 RO2-N. + #.344 R2O2. + #.558 RCO-O2. + #.005 CO + #.225 RCHO + #.008 MGLY + #-0.634 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.161 HO2. + #1.359 RO2-R. + #.48 RO2-N. + CO + #.452 RCHO + #.069 PROD2 + #-2.645 XC
1-Pentadecene [LP]	3.16e-11	3.16e-11			1-C15E + HO. = #.629 RO2-R. + #.371 RO2-N. + #.388 R2O2. + #.372 HCHO + #.43 RCHO + #.2 PROD2 + #9.917 XC
	1.01e-17	1.01e-17			1-C15E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 RCHO + #.5 PROD2 + #.185 HCOOH + #9.5 XC
	1.38e-14	1.38e-14			1-C15E + NO3 = #.525 RO2-R. + #.475 RO2-N. + #.771 R2O2. + #.525 RNO3 + #9 XC + #.475 XN
	5.60e-12	5.60e-12			1-C15E + O3P = #.45 RCHO + #.55 PROD2 + #10.35 XC
1-Pentadecene [AP]	3.16e-11	3.16e-11			1-C15E + HO. = #.629 RO2-R. + #.371 RO2-N. + #.388 R2O2. + #.372 HCHO + #9.917 XC + #.43 PRD1 + #.2 PRD2
	1.01e-17	1.01e-17			1-C15E + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #9.5 XC + #.5 PRD3 + #.5 PRD4
	1.38e-14	1.38e-14			1-C15E + NO3 = #.525 RO2-R. + #.475 RO2-N. + #.771 R2O2. + #.525 RNO3 + #9 XC + #.475 XN
	5.60e-12	5.60e-12			1-C15E + O3P = #10.35 XC + #.55 PRD5 + #.45 PRD6
	3.77e-11	3.77e-11			PRD1 + HO. = #.02 HO2. + #.248 RO2-R. + #.198 RO2-N. + #.298 R2O2. + #.533 RCO-O2. + #.004 CO + #.246 RCHO + #.026 MGLY + #-0.612 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.407 HO2. + #1.178 RO2-R. + #.415 RO2-N. + CO + #.525 RCHO + #.06 PROD2 + #-2.425 XC
	3.14e-11	3.14e-11			PRD2 + HO. = #.112 HO2. + #.618 RO2-R. + #.225 RO2-N. + #.045 RCO-O2. + #.018 HCHO + #.301 RCHO + #.514 PROD2 + #.079 MGLY + #.273 XC
	3.56e-11	3.56e-11			PRD3 + HO. = #.233 RO2-R. + #.21 RO2-N. + #.344 R2O2. + #.558 RCO-O2. + #.005 CO + #.225 RCHO + #.008 MGLY + #-0.634 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.161 HO2. + #1.359 RO2-R. + #.48 RO2-N. + CO + #.452 RCHO + #.069 PROD2 + #-2.645 XC
	1.95e-11	1.95e-11			PRD4 + HO. = #.533 RO2-R. + #.467 RO2-N. + #.765 R2O2. + #.512 PROD2 + #.021 BACL + #.041 XC
	1.76e-11	1.76e-11			PRD5 + HO. = #.493 RO2-R. + #.504 RO2-N. + #1.015 R2O2. + #.003 RCO-O2. + #.046 CO + #.004 CO2 + #.004 HCHO + #.064 RCHO + #.429 PROD2 + #.001 BACL + #.028 HCOOH + #.079 XC
	3.70e-11	3.70e-11			PRD6 + HO. = #.243 RO2-R. + #.221 RO2-N. + #.36 R2O2. + #.536 RCO-O2. + #.005 CO + #.235 RCHO + #.008 MGLY + #-0.668 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.166 HO2. + #1.349 RO2-R. + #.485 RO2-N. + CO + #.447 RCHO + #.068 PROD2 + #-2.659 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Isobutene [LP]	5.14e-11	9.47e-12	-1.00		ISOBUTEN + HO. = #.9 RO2-R. + #.1 RO2-N. + #.9 HCHO + #.9 ACET + #-0.2 XC
	1.13e-17	2.70e-15	3.24		ISOBUTEN + O3 = #.707 HO. + #.04 RO2-R. + #.627 R2O2. + #.667 CCO-O2. + #.167 CO + #.043 CO2 + #1.333 HCHO + #.333 ACET + #.123 HCOOH
	3.32e-13	3.32e-13			ISOBUTEN + NO3 = #.644 NO2 + #.039 RO2-N. + #.961 R2O2. + #.316 C-O2. + #.644 HCHO + #.644 ACET + #.87 XC + #.356 XN
	1.69e-11	1.69e-11			ISOBUTEN + O3P = #.4 RCHO + #.6 MEK + #.4 XC
Isobutene [AP]	5.14e-11	9.47e-12	-1.00		ISOBUTEN + HO. = #.9 RO2-R. + #.1 RO2-N. + #.9 HCHO + #.9 ACET + #-0.2 XC
	1.13e-17	2.70e-15	3.24		ISOBUTEN + O3 = #.707 HO. + #.04 RO2-R. + #.627 R2O2. + #.667 CCO-O2. + #.167 CO + #.043 CO2 + #1.333 HCHO + #.333 ACET + #.123 HCOOH
	3.32e-13	3.32e-13			ISOBUTEN + NO3 = #.644 NO2 + #.039 RO2-N. + #.961 R2O2. + #.316 C-O2. + #.644 HCHO + #.644 ACET + #.87 XC + #.356 XN
	1.69e-11	1.69e-11			ISOBUTEN + O3P = #.6 MEK + #.4 XC + #.4 PRD1
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
2-Methyl-1-Butene [LP]	6.11e-11	1.14e-11	-0.99		2M-1-BUT + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 HCHO + #.935 MEK + #-0.065 XC
	1.60e-17	2.70e-15	3.04		2M-1-BUT + O3 = #.707 HO. + #.04 RO2-R. + #.026 RO2-N. + #.6 R2O2. + #.558 CCO-O2. + #.082 RCO-O2. + #.167 CO + #.043 CO2 + #.749 HCHO + #.558 CCHO + #.333 MEK + #.123 HCOOH + #-0.053 XC
	3.32e-13	3.32e-13			2M-1-BUT + NO3 = #.019 NO2 + #.916 RO2-R. + #.065 RO2-N. + #.935 R2O2. + #.019 HCHO + #.916 CCHO + #.019 MEK + #2.682 XC + #.981 XN
	1.87e-11	1.87e-11			2M-1-BUT + O3P = #.4 RCHO + #.6 MEK + #1.4 XC
2-Methyl-1-Butene [AP]	6.11e-11	1.14e-11	-0.99		2M-1-BUT + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 HCHO + #.935 MEK + #-0.065 XC
	1.60e-17	2.70e-15	3.04		2M-1-BUT + O3 = #.707 HO. + #.04 RO2-R. + #.026 RO2-N. + #.6 R2O2. + #.558 CCO-O2. + #.082 RCO-O2. + #.167 CO + #.043 CO2 + #.749 HCHO + #.558 CCHO + #.333 MEK + #.123 HCOOH + #-0.053 XC
	3.32e-13	3.32e-13			2M-1-BUT + NO3 = #.019 NO2 + #.916 RO2-R. + #.065 RO2-N. + #.935 R2O2. + #.019 HCHO + #.916 CCHO + #.019 MEK + #2.682 XC + #.981 XN
	1.87e-11	1.87e-11			2M-1-BUT + O3P = #.6 MEK + #1.4 XC + #.4 PRD1
	2.25e-11	2.25e-11			PRD1 + HO. = #.119 RO2-R. + #.014 RO2-N. + #.046 R2O2. + #.867 RCO-O2. + #.119 CO + #.09 CCHO + #.076 MEK + #-0.284 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.637 HO2. + #1.282 RO2-R. + #.08 RO2-N. + CO + #.725 CCHO + #.557 MEK + #-2.161 XC
23-Dimethyl-1-Butene [LP]	5.79e-11	5.79e-11			23M1-BUT + HO. = #.899 RO2-R. + #.101 RO2-N. + #.074 R2O2. + #.828 HCHO + #.071 ACET + #.902 MEK + #.746 XC
	1.30e-17	2.70e-15	3.16		23M1-BUT + O3 = #.707 HO. + #.04 RO2-R. + #.043 RO2-N. + #.583 R2O2. + #.582 CCO-O2. + #.042 RCO-O2. + #.167 CO + #.043 CO2 + #.708 HCHO + #.582 ACET + #.333 MEK + #.123 HCOOH + #.332 XC
	3.32e-13	3.32e-13			23M1-BUT + NO3 = #.866 RO2-R. + #.134 RO2-N. + #.902 R2O2. + #.866 ACET + #2.599 XC + XN
	1.73e-11	1.73e-11			23M1-BUT + O3P = #.4 RCHO + #.6 MEK + #2.4 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
23-Dimethyl-1-Butene [AP]	5.79e-11	5.79e-11			23M1-BUT + HO. = #.899 RO2-R. + #.101 RO2-N. + #.074 R2O2. + #.828 HCHO + #.071 ACET + #.902 MEK + #.746 XC
	1.30e-17	2.70e-15	3.16		23M1-BUT + O3 = #.707 HO. + #.04 RO2-R. + #.043 RO2-N. + #.583 R2O2. + #.582 CCO-O2. + #.042 RCO-O2. + #.167 CO + #.043 CO2 + #.708 HCHO + #.582 ACET + #.333 MEK + #.123 HCOOH + #.332 XC
	3.32e-13	3.32e-13			23M1-BUT + NO3 = #.866 RO2-R. + #.134 RO2-N. + #.902 R2O2. + #.866 ACET + #2.599 XC + XN
	1.73e-11	1.73e-11			23M1-BUT + O3P = #.6 MEK + #2.4 XC + #.4 PRD1
	2.39e-11	2.39e-11			PRD1 + HO. = #.155 RO2-R. + #.023 RO2-N. + #.104 R2O2. + #.822 RCO-O2. + #.154 CO + #.086 CCHO + #.091 ACET + #.068 MEK + #-0.479 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.169 HO2. + #1.657 RO2-R. + #.174 RO2-N. + CO + #.831 CCHO + #.798 ACET + #.028 MEK + #-3.213 XC
2-Ethyl-1-Butene [LP]	5.79e-11	5.79e-11			2E1-BUT + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 HCHO + #.902 MEK + #.902 XC
	1.30e-17	2.70e-15	3.16		2E1-BUT + O3 = #.707 HO. + #.04 RO2-R. + #.043 RO2-N. + #.583 R2O2. + #.623 RCO-O2. + #.167 CO + #.043 CO2 + #.667 HCHO + #.623 CCHO + #.333 MEK + #.123 HCOOH + #.29 XC
	3.32e-13	3.32e-13			2E1-BUT + NO3 = #.009 NO2 + #.893 RO2-R. + #.098 RO2-N. + #.902 R2O2. + #.009 HCHO + #.893 CCHO + #.009 MEK + #.893 RNO3 + #-1.776 XC + #.098 XN
	1.73e-11	1.73e-11			2E1-BUT + O3P = #.4 RCHO + #.6 MEK + #2.4 XC
2-Ethyl-1-Butene [AP]	5.79e-11	5.79e-11			2E1-BUT + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 HCHO + #.902 MEK + #.902 XC
	1.30e-17	2.70e-15	3.16		2E1-BUT + O3 = #.707 HO. + #.04 RO2-R. + #.043 RO2-N. + #.583 R2O2. + #.623 RCO-O2. + #.167 CO + #.043 CO2 + #.667 HCHO + #.623 CCHO + #.333 MEK + #.123 HCOOH + #.29 XC
	3.32e-13	3.32e-13			2E1-BUT + NO3 = #.009 NO2 + #.893 RO2-R. + #.098 RO2-N. + #.902 R2O2. + #.009 HCHO + #.893 CCHO + #.009 MEK + #.893 RNO3 + #-1.776 XC + #.098 XN
	1.73e-11	1.73e-11			2E1-BUT + O3P = #.6 MEK + #2.4 XC + #.4 PRD1
	2.41e-11	2.41e-11			PRD1 + HO. = #.162 RO2-R. + #.032 RO2-N. + #.096 R2O2. + #.806 RCO-O2. + #.158 CO + #.082 CCHO + #.079 RCHO + #.082 MEK + #-0.5 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.625 HO2. + #1.259 RO2-R. + #.116 RO2-N. + CO + #.375 CCHO + #.375 RCHO + #.509 MEK + #-2.607 XC
2-Methyl-1-Pentene [LP]	6.32e-11	1.18e-11	-0.99		2M1-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 HCHO + #.902 MEK + #.902 XC
	1.50e-17	2.70e-15	3.08		2M1-C5E + O3 = #.707 HO. + #.04 RO2-R. + #.043 RO2-N. + #.583 R2O2. + #.556 CCO-O2. + #.067 RCO-O2. + #.167 CO + #.043 CO2 + #.734 HCHO + #.556 RCHO + #.333 MEK + #.123 HCOOH + #.357 XC
	3.32e-13	3.32e-13			2M1-C5E + NO3 = #.827 RO2-R. + #.173 RO2-N. + #.902 R2O2. + #.827 RCHO + #2.48 XC + XN
	2.00e-11	2.00e-11			2M1-C5E + O3P = #.4 RCHO + #.6 MEK + #2.4 XC
2-Methyl-1-Pentene [AP]	6.32e-11	1.18e-11	-0.99		2M1-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 HCHO + #.902 MEK + #.902 XC
	1.50e-17	2.70e-15	3.08		2M1-C5E + O3 = #.707 HO. + #.04 RO2-R. + #.043 RO2-N. + #.583 R2O2. + #.556 CCO-O2. + #.067 RCO-O2. + #.167 CO + #.043 CO2 + #.734 HCHO + #.556 RCHO + #.333 MEK + #.123 HCOOH + #.357 XC
	3.32e-13	3.32e-13			2M1-C5E + NO3 = #.827 RO2-R. + #.173 RO2-N. + #.902 R2O2. + #.156 RCHO + #2.48 XC + #.67 PRD1 + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.00e-11	2.00e-11			2M1-C5E + O3P = #.6 MEK + #2.4 XC + #.4 PRD2
	2.19e-11	2.19e-11			PRD1 + HO. = #.001 NO2 + #.095 RO2-R. + #.011 RO2-N. + #.003 R2O2. + #.894 RCO-O2. + #.033 CO + #.002 HCHO + #.095 RCHO + #.001 MGLY + #-0.067 XC + #.999 XN
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD1 + HV = #.161 NO2 + #.206 HO2. + #1.526 RO2-R. + #.106 RO2-N. + CO + #.465 HCHO + #.429 RCHO + #.465 RNO3 + #-3.177 XC + #.374 XN
	2.39e-11	2.39e-11			PRD2 + HO. = #.118 RO2-R. + #.027 RO2-N. + #.092 R2O2. + #.855 RCO-O2. + #.117 CO + #.048 CCHO + #.052 RCHO + #.069 MEK + #-0.371 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.223 HO2. + #1.612 RO2-R. + #.165 RO2-N. + CO + #.029 CCHO + #.029 RCHO + #.107 MEK + #.699 PROD2 + #-3.758 XC
2,3,3-trimethyl-1-Butene [LP]	5.79e-11	5.79e-11			233M1BUT + HO. = #.082 RO2-R. + #.166 RO2-N. + #1.534 R2O2. + #.752 TBU-O. + #.082 HCHO + #.865 MEK + #.207 XC
	8.30e-18	2.70e-15	3.43		233M1BUT + O3 = #.707 HO. + #.04 RO2-R. + #.065 RO2-N. + #.562 R2O2. + #.602 RCO-O2. + #.167 CO + #.043 CO2 + #1.268 HCHO + #.333 MEK + #.123 HCOOH + #1.87 XC
	3.32e-13	3.32e-13			233M1BUT + NO3 = #.169 RO2-N. + #1.696 R2O2. + #.831 TBU-O. + #3.492 XC + XN
	1.73e-11	1.73e-11			233M1BUT + O3P = #.4 RCHO + #.6 MEK + #3.4 XC
2,3,3-trimethyl-1-Butene [AP]	5.79e-11	5.79e-11			233M1BUT + HO. = #.082 RO2-R. + #.166 RO2-N. + #1.534 R2O2. + #.752 TBU-O. + #.082 HCHO + #.865 MEK + #.207 XC
	8.30e-18	2.70e-15	3.43		233M1BUT + O3 = #.707 HO. + #.04 RO2-R. + #.065 RO2-N. + #.562 R2O2. + #.602 RCO-O2. + #.167 CO + #.043 CO2 + #1.268 HCHO + #.333 MEK + #.123 HCOOH + #1.87 XC
	3.32e-13	3.32e-13			233M1BUT + NO3 = #.169 RO2-N. + #1.696 R2O2. + #.831 TBU-O. + #3.492 XC + XN
	1.73e-11	1.73e-11			233M1BUT + O3P = #.6 MEK + #3.4 XC + #.4 PRD1
	2.17e-11	2.17e-11			PRD1 + HO. = #.052 RO2-R. + #.017 RO2-N. + #.083 R2O2. + #.904 RCO-O2. + #.027 TBU-O. + #.052 CO + #.009 HCHO + #.008 CCHO + #.008 ACET + #.044 MEK + #.028 MGLY + #-0.256 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = RO2-R. + #.188 RO2-N. + #.658 R2O2. + #.812 TBU-O. + CO + #.845 CCHO + #-3.255 XC
3-Methyl-2-Isopropyl-1-Butene [LP]	5.79e-11	5.79e-11			3M2I1C4E + HO. = #.822 RO2-R. + #.178 RO2-N. + #.125 R2O2. + #.701 HCHO + #.12 ACET + #.827 PROD2 + #.908 XC
	3.30e-18	2.70e-15	3.97		3M2I1C4E + O3 = #.707 HO. + #.04 RO2-R. + #.09 RO2-N. + #.537 R2O2. + #.577 RCO-O2. + #.167 CO + #.043 CO2 + #.667 HCHO + #.577 ACET + #.333 PROD2 + #.123 HCOOH + XC
	3.32e-13	3.32e-13			3M2I1C4E + NO3 = #.794 RO2-R. + #.206 RO2-N. + #.827 R2O2. + #.794 ACET + #.827 RNO3 + #-0.579 XC + #.173 XN
	1.73e-11	1.73e-11			3M2I1C4E + O3P = #.4 RCHO + #.6 PROD2 + #3.2 XC
3-Methyl-2-Isopropyl-1-Butene [AP]	5.79e-11	5.79e-11			3M2I1C4E + HO. = #.822 RO2-R. + #.178 RO2-N. + #.125 R2O2. + #.701 HCHO + #.12 ACET + #.908 XC + #.827 PRD1
	3.30e-18	2.70e-15	3.97		3M2I1C4E + O3 = #.707 HO. + #.04 RO2-R. + #.09 RO2-N. + #.537 R2O2. + #.577 RCO-O2. + #.167 CO + #.043 CO2 + #.667 HCHO + #.577 ACET + #.123 HCOOH + XC + #.333 PRD2
	3.32e-13	3.32e-13			3M2I1C4E + NO3 = #.794 RO2-R. + #.206 RO2-N. + #.827 R2O2. + #.794 ACET + #.827 RNO3 + #-0.579 XC + #.173 XN
	1.73e-11	1.73e-11			3M2I1C4E + O3P = #3.2 XC + #.6 PRD3 + #.4 PRD4

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	5.40e-12	5.40e-12			PRD1 + HO. = #.157 RO2-R. + #.143 RO2-N. + #.867 R2O2. + #.7 RCO-O2. + #.253 HCHO + #.216 CCHO + #.087 RCHO + #.469 ACET + #.07 MGLY + #.479 XC
	PF=KETONE QY = 2.5e-2				PRD1 + HV = #.151 HO2. + #.815 RO2-R. + #.034 RO2-N. + RCO-O2. + #.151 HCHO + #.815 ACET + #.201 XC
	5.38e-12	5.38e-12			PRD2 + HO. = #.095 RO2-R. + #.162 RO2-N. + #1.015 R2O2. + #.743 RCO-O2. + #.259 HCHO + #.234 CCHO + #.095 RCHO + #.509 ACET + #.259 XC
	PF=KETONE QY = 2.0e-2				PRD2 + HV = #.96 RO2-R. + #.04 RO2-N. + RCO-O2. + #.96 ACET + #-0.12 XC
	5.64e-12	5.64e-12			PRD3 + HO. = #.696 RO2-R. + #.302 RO2-N. + #1.7 R2O2. + #.002 RCO-O2. + #.224 CO + #.005 CO2 + #.052 HCHO + #.052 CCHO + #.734 ACET + #.458 MEK + #.018 PROD2 + #.222 RCO-OH + #-1.012 XC
	2.69e-11	2.69e-11			PRD4 + HO. = #.207 RO2-R. + #.069 RO2-N. + #.178 R2O2. + #.724 RCO-O2. + #.206 CO + #.139 RCHO + #.157 ACET + #.067 PROD2 + #.001 MGLY + #-1.085 XC
	3.80e-15	3.80e-15			PRD4 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD4 + HV = #.209 HO2. + #1.568 RO2-R. + #.223 RO2-N. + CO + #.791 RCHO + #.759 ACET + #.018 PROD2 + #-4.095 XC
cis-2-Butene	5.64e-11	1.10e-11	-0.97		C-2-BUTE + HO. = #.965 RO2-R. + #.035 RO2-N. + #1.93 CCHO + #-0.07 XC
	1.25e-16	3.22e-15	1.92		C-2-BUTE + O3 = #.52 HO. + #.52 C-O2. + #.52 CO + #.14 CO2 + CCHO + #.34 CCO-OH + #.14 INERT + #.14 XC
	3.51e-13	1.10e-13	-0.69		C-2-BUTE + NO3 = #.705 NO2 + #.215 RO2-R. + #.08 RO2-N. + #.705 R2O2. + #1.41 CCHO + #.215 RNO3 + #-0.59 XC + #.08 XN
	1.76e-11	1.76e-11			C-2-BUTE + O3P = MEK
trans-2-Butene	6.40e-11	1.01e-11	-1.09		T-2-BUTE + HO. = #.965 RO2-R. + #.035 RO2-N. + #1.93 CCHO + #-0.07 XC
	1.90e-16	6.64e-15	2.10		T-2-BUTE + O3 = #.52 HO. + #.52 C-O2. + #.52 CO + #.14 CO2 + CCHO + #.34 CCO-OH + #.14 INERT + #.14 XC
	3.91e-13	1.10e-13	-0.76	2.0	T-2-BUTE + NO3 = #.705 NO2 + #.215 RO2-R. + #.08 RO2-N. + #.705 R2O2. + #1.41 CCHO + #.215 RNO3 + #-0.59 XC + #.08 XN
	2.18e-11	2.18e-11			T-2-BUTE + O3P = MEK
2-Methyl-2-Butene	8.69e-11	1.92e-11	-0.89		2M-2-BUT + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 CCHO + #.935 ACET + #-0.065 XC
	4.03e-16	2.87e-15	1.16		2M-2-BUT + O3 = #.856 HO. + #.7 R2O2. + #.156 C-O2. + #.7 CCO-O2. + #.156 CO + #.042 CO2 + #.7 HCHO + #.7 CCHO + #.3 ACET + #.102 CCO-OH + #.042 INERT + #.042 XC
	9.37e-12	9.37e-12			2M-2-BUT + NO3 = #.935 NO2 + #.065 RO2-N. + #.935 R2O2. + #.935 CCHO + #.935 ACET + #-0.065 XC + #.065 XN
	5.10e-11	5.10e-11			2M-2-BUT + O3P = MEK + XC
cis-2-Pentene	6.48e-11	1.21e-11	-0.99		C-2-PENT + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 CCHO + #.935 RCHO + #-0.065 XC
	1.15e-16	1.15e-16			C-2-PENT + O3 = #.317 HO. + #.057 RO2-R. + #.26 C-O2. + #.317 CO + #.07 CO2 + #.556 CCHO + #.5 RCHO + #.17 CCO-OH + #.444 RCO-OH + #.07 INERT + #.07 XC
	3.70e-13	3.70e-13			C-2-PENT + NO3 = #.471 NO2 + #.395 RO2-R. + #.134 RO2-N. + #.753 R2O2. + #.481 CCHO + #.481 RCHO + #.386 RNO3 + #-0.519 XC + #.143 XN
	1.70e-11	1.70e-11			C-2-PENT + O3P = MEK + XC
trans-2-Pentene	6.70e-11	1.25e-11	-0.99		T-2-PENT + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 CCHO + #.935 RCHO + #-0.065 XC
	1.15e-16	1.15e-16			T-2-PENT + O3 = #.317 HO. + #.057 RO2-R. + #.26 C-O2. + #.317 CO + #.07 CO2 + #.556 CCHO + #.5 RCHO + #.17 CCO-OH + #.444 RCO-OH + #.07 INERT + #.07 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.70e-13	3.70e-13			T-2-PENT + NO3 = #.471 NO2 + #.395 RO2-R. + #.134 RO2-N. + #.753 R2O2. + #.481 CCHO + #.481 RCHO + #.386 RNO3 + #-0.519 XC + #.143 XN
	2.23e-11	2.23e-11			T-2-PENT + O3P = MEK + XC
2,3-Dimethyl-2-Butene	1.10e-10	2.05e-11	-0.99		23M2-BUT + HO. = #.902 RO2-R. + #.098 RO2-N. + #1.805 ACET + #-0 XC
	1.13e-15	3.03e-15	0.58		23M2-BUT + O3 = HO. + R2O2. + CCO-O2. + HCHO + ACET
	5.72e-11	5.72e-11			23M2-BUT + NO3 = #.902 NO2 + #.098 RO2-N. + #.902 R2O2. + #1.805 ACET + #-0 XC + #.098 XN
	7.64e-11	7.64e-11			23M2-BUT + O3P = MEK + #2 XC
2-Methyl-2-Pentene [LP]	8.89e-11	1.66e-11	-0.99		2M-2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 RCHO + #.902 ACET
	3.48e-16	3.48e-16			2M-2-C5E + O3 = #.734 HO. + #.034 RO2-R. + #.7 R2O2. + #.7 CCO-O2. + #.034 CO + #.7 HCHO + #.034 CCHO + #.7 RCHO + #.3 ACET + #.266 RCO-OH
	9.37e-12	9.37e-12			2M-2-C5E + NO3 = #.391 NO2 + #.46 RO2-R. + #.149 RO2-N. + #.92 R2O2. + #.016 HCHO + #.845 RCHO + #.391 ACET + #.006 RNO3 + #1.346 XC + #.602 XN
	3.78e-11	3.78e-11			2M-2-C5E + O3P = MEK + #2 XC
2-Methyl-2-Pentene [AP]	8.89e-11	1.66e-11	-0.99		2M-2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 RCHO + #.902 ACET
	3.48e-16	3.48e-16			2M-2-C5E + O3 = #.734 HO. + #.034 RO2-R. + #.7 R2O2. + #.7 CCO-O2. + #.034 CO + #.7 HCHO + #.034 CCHO + #.7 RCHO + #.3 ACET + #.266 RCO-OH
	9.37e-12	9.37e-12			2M-2-C5E + NO3 = #.391 NO2 + #.46 RO2-R. + #.149 RO2-N. + #.92 R2O2. + #.016 HCHO + #.391 RCHO + #.391 ACET + #.006 RNO3 + #1.346 XC + #.454 PRD1 + #.602 XN
	3.78e-11	3.78e-11			2M-2-C5E + O3P = MEK + #2 XC
	2.07e-11	2.07e-11			PRD1 + HO. = #.052 RO2-R. + #.007 RO2-N. + #.011 R2O2. + #.941 RCO-O2. + #.028 CO + #.022 HCHO + #.051 RCHO + #.002 MGLY + #-0.071 XC + XN
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD1 + HV = #.024 NO2 + #.131 HO2. + #1.725 RO2-R. + #.12 RO2-N. + CO + #.691 HCHO + #.213 RCHO + #.667 RNO3 + #-4.051 XC + #.309 XN
Cis-2-Hexene [LP]	6.34e-11	6.34e-11			C-2-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 RCHO + #.902 XC
	1.15e-16	1.15e-16			C-2-C6E + O3 = #.301 HO. + #.04 RO2-R. + #.001 RO2-N. + #.26 C-O2. + #.301 CO + #.07 CO2 + #.5 CCHO + #.54 RCHO + #.17 CCO-OH + #.46 RCO-OH + #.07 INERT + #1.025 XC
	3.70e-13	3.70e-13			C-2-C6E + NO3 = #.12 NO2 + #.659 RO2-R. + #.221 RO2-N. + #.807 R2O2. + #.12 CCHO + #.134 RCHO + #.652 RNO3 + #.12 XC + #.228 XN
	2.05e-11	2.05e-11			C-2-C6E + O3P = #.76 MEK + #.24 PROD2 + #1.52 XC
Cis-2-Hexene [AP]	6.34e-11	6.34e-11			C-2-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 XC + #.902 PRD1
	1.15e-16	1.15e-16			C-2-C6E + O3 = #.301 HO. + #.04 RO2-R. + #.001 RO2-N. + #.26 C-O2. + #.301 CO + #.07 CO2 + #.5 CCHO + #.04 RCHO + #.17 CCO-OH + #.46 RCO-OH + #.07 INERT + #1.025 XC + #.5 PRD1
	3.70e-13	3.70e-13			C-2-C6E + NO3 = #.12 NO2 + #.659 RO2-R. + #.221 RO2-N. + #.807 R2O2. + #.12 CCHO + #.007 RCHO + #.652 RNO3 + #.12 XC + #.127 PRD2 + #.228 XN
	2.05e-11	2.05e-11			C-2-C6E + O3P = #.76 MEK + #1.52 XC + #.24 PRD3
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	2.33e-11	2.33e-11			PRD2 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	7.51e-12	7.51e-12			PRD3 + HO. = #.434 RO2-R. + #.106 RO2-N. + #.839 R2O2. + #.23 CCO-O2. + #.23 RCO-O2. + #.24 HCHO + #.253 CCHO + #.445 RCHO + #.245 MEK + #.044 PROD2 + #.891 XC
		PF=KETONE QY = 5.0e-2			PRD3 + HV = #.955 RO2-R. + #.045 RO2-N. + #.377 R2O2. + #.5 CCO-O2. + #.5 RCO-O2. + #.955 RCHO + #.366 XC
Cis-3-Hexene [LP]	6.34e-11	6.34e-11			C-3-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #1.805 RCHO
	1.50e-16	3.22e-15	1.82		C-3-C6E + O3 = #.113 HO. + #.113 RO2-R. + #.113 CO + #.113 CCHO + RCHO + #.887 RCO-OH + #-0 XC
	3.70e-13	3.70e-13			C-3-C6E + NO3 = #.284 NO2 + #.514 RO2-R. + #.202 RO2-N. + #.774 R2O2. + #.567 RCHO + #.514 RNO3 + #.202 XN
	2.05e-11	2.05e-11			C-3-C6E + O3P = #.76 MEK + #.24 PROD2 + #1.52 XC
Cis-3-Hexene [AP]	6.34e-11	6.34e-11			C-3-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #1.805 RCHO
	1.50e-16	3.22e-15	1.82		C-3-C6E + O3 = #.113 HO. + #.113 RO2-R. + #.113 CO + #.113 CCHO + RCHO + #.887 RCO-OH + #-0 XC
	3.70e-13	3.70e-13			C-3-C6E + NO3 = #.284 NO2 + #.514 RO2-R. + #.202 RO2-N. + #.774 R2O2. + #.567 RCHO + #.514 RNO3 + #.202 XN
	2.05e-11	2.05e-11			C-3-C6E + O3P = #.76 MEK + #1.52 XC + #.24 PRD1
	5.92e-12	5.92e-12			PRD1 + HO. = #.445 RO2-R. + #.11 RO2-N. + #.663 R2O2. + #.445 RCO-O2. + #.141 HCHO + #.312 CCHO + #.24 RCHO + #.344 MEK + #1.142 XC
		PF=KETONE QY = 5.0e-2			PRD1 + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #-0.06 XC
Cis-3-Methyl-2-Hexene [LP]	8.71e-11	8.71e-11			C3M2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 MEK + #-0 XC
	4.51e-16	2.87e-15	1.10		C3M2-C5E + O3 = #.856 HO. + #.028 RO2-N. + #.672 R2O2. + #.156 C-O2. + #.586 CCO-O2. + #.087 RCO-O2. + #.156 CO + #.042 CO2 + #.087 HCHO + #1.286 CCHO + #.3 MEK + #.102 CCO-OH + #.042 INERT + #-0.013 XC
	9.37e-12	9.37e-12			C3M2-C5E + NO3 = #.872 NO2 + #.03 RO2-R. + #.098 RO2-N. + #.902 R2O2. + #.902 CCHO + #.872 MEK + #.03 RNO3 + #-0.06 XC + #.098 XN
	3.71e-11	3.71e-11			C3M2-C5E + O3P = #.6 MEK + #.4 PROD2 + #1.2 XC
Cis-3-Methyl-2-Hexene [AP]	8.71e-11	8.71e-11			C3M2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 MEK + #-0 XC
	4.51e-16	2.87e-15	1.10		C3M2-C5E + O3 = #.856 HO. + #.028 RO2-N. + #.672 R2O2. + #.156 C-O2. + #.586 CCO-O2. + #.087 RCO-O2. + #.156 CO + #.042 CO2 + #.087 HCHO + #1.286 CCHO + #.3 MEK + #.102 CCO-OH + #.042 INERT + #-0.013 XC
	9.37e-12	9.37e-12			C3M2-C5E + NO3 = #.872 NO2 + #.03 RO2-R. + #.098 RO2-N. + #.902 R2O2. + #.902 CCHO + #.872 MEK + #.03 RNO3 + #-0.06 XC + #.098 XN
	3.71e-11	3.71e-11			C3M2-C5E + O3P = #.6 MEK + #1.2 XC + #.4 PRD1
	6.24e-12	6.24e-12			PRD1 + HO. = #.059 RO2-R. + #.126 RO2-N. + #1.43 R2O2. + #.801 CCO-O2. + #.015 RCO-O2. + #.054 HCHO + #1.031 CCHO + #.095 RCHO + #.259 MEK + #.162 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=KETONE QY = 5.0e-2				PRD1 + HV = #.92 RO2-R. + #.08 RO2-N. + #.363 R2O2. + CCO-O2. + #.725 CCHO + #.557 MEK + #-0.161 XC
Trans 3-Methyl-2-Hexene [LP]	8.71e-11	8.71e-11			T3M2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 MEK + #-0 XC
	5.61e-16	2.87e-15	0.97		T3M2-C5E + O3 = #.856 HO. + #.028 RO2-N. + #.672 R2O2. + #.156 C-O2. + #.586 CCO-O2. + #.087 RCO-O2. + #.156 CO + #.042 CO2 + #.087 HCHO + #1.286 CCHO + #.3 MEK + #.102 CCO-OH + #.042 INERT + #-0.013 XC
	9.37e-12	9.37e-12			T3M2-C5E + NO3 = #.872 NO2 + #.03 RO2-R. + #.098 RO2-N. + #.902 R2O2. + #.902 CCHO + #.872 MEK + #.03 RNO3 + #-0.06 XC + #.098 XN
	3.71e-11	3.71e-11			T3M2-C5E + O3P = #.6 MEK + #.4 PROD2 + #1.2 XC
Trans 3-Methyl-2-Hexene [AP]	8.71e-11	8.71e-11			T3M2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 MEK + #-0 XC
	5.61e-16	2.87e-15	0.97		T3M2-C5E + O3 = #.856 HO. + #.028 RO2-N. + #.672 R2O2. + #.156 C-O2. + #.586 CCO-O2. + #.087 RCO-O2. + #.156 CO + #.042 CO2 + #.087 HCHO + #1.286 CCHO + #.3 MEK + #.102 CCO-OH + #.042 INERT + #-0.013 XC
	9.37e-12	9.37e-12			T3M2-C5E + NO3 = #.872 NO2 + #.03 RO2-R. + #.098 RO2-N. + #.902 R2O2. + #.902 CCHO + #.872 MEK + #.03 RNO3 + #-0.06 XC + #.098 XN
	3.71e-11	3.71e-11			T3M2-C5E + O3P = #.6 MEK + #1.2 XC + #.4 PRD1
	6.24e-12	6.24e-12			PRD1 + HO. = #.059 RO2-R. + #.126 RO2-N. + #1.43 R2O2. + #.801 CCO-O2. + #.015 RCO-O2. + #.054 HCHO + #1.031 CCHO + #.095 RCHO + #.259 MEK + #.162 XC
	PF=KETONE QY = 5.0e-2				PRD1 + HV = #.92 RO2-R. + #.08 RO2-N. + #.363 R2O2. + CCO-O2. + #.725 CCHO + #.557 MEK + #-0.161 XC
Trans 4-Methyl-2-Hexene [LP]	6.11e-11	1.14e-11	-0.99		T4M2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.017 R2O2. + #.885 CCHO + #.902 RCHO + #.016 ACET + #.883 XC
	1.15e-16	1.15e-16			T4M2-C5E + O3 = #.301 HO. + #.039 RO2-R. + #.002 RO2-N. + #.26 C-O2. + #.301 CO + #.07 CO2 + #.5 CCHO + #.5 RCHO + #.039 ACET + #.17 CCO-OH + #.46 RCO-OH + #.07 INERT + #1.023 XC
	3.70e-13	3.70e-13			T4M2-C5E + NO3 = #.197 NO2 + #.611 RO2-R. + #.192 RO2-N. + #.807 R2O2. + #.197 CCHO + #.585 RCHO + #.373 ACET + #.238 RNO3 + #.151 XC + #.564 XN
	1.87e-11	1.87e-11			T4M2-C5E + O3P = #.88 MEK + #.12 PROD2 + #1.76 XC
Trans 4-Methyl-2-Hexene [AP]	6.11e-11	1.14e-11	-0.99		T4M2-C5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.017 R2O2. + #.885 CCHO + #.016 ACET + #.883 XC + #.902 PRD1
	1.15e-16	1.15e-16			T4M2-C5E + O3 = #.301 HO. + #.039 RO2-R. + #.002 RO2-N. + #.26 C-O2. + #.301 CO + #.07 CO2 + #.5 CCHO + #.039 ACET + #.17 CCO-OH + #.46 RCO-OH + #.07 INERT + #1.023 XC + #.5 PRD2
	3.70e-13	3.70e-13			T4M2-C5E + NO3 = #.197 NO2 + #.611 RO2-R. + #.192 RO2-N. + #.807 R2O2. + #.197 CCHO + #.373 ACET + #.238 RNO3 + #.151 XC + #.585 PRD3 + #.564 XN
	1.87e-11	1.87e-11			T4M2-C5E + O3P = #.88 MEK + #1.76 XC + #.12 PRD4
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	2.60e-11	2.60e-11			PRD2 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD2 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	2.17e-11	2.17e-11			PRD3 + HO. = #.028 RO2-R. + #.001 RO2-N. + #.004 R2O2. + #.971 RCO-O2. + #.026 CO + #.004 HCHO + #.004 CCHO + #.001 RCHO + #.022 ACET + #-0.03 XC + #.663 XN
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + #-0 XC + #1.663 XN
		PF=C2CHO			PRD3 + HV = #.663 NO2 + HO2. + #.323 RO2-R. + #.013 RO2-N. + CO + #.663 CCHO + #.323 ACET + #-0.377 XC
	1.41e-11	1.41e-11			PRD4 + HO. = #.012 RO2-R. + #.099 RO2-N. + #1.706 R2O2. + #.878 CCO-O2. + #.011 RCO-O2. + #.827 HCHO + #.021 CCHO + #.096 RCHO + #.768 ACET + #.004 MEK + #.135 XC
		PF=KETONE QY = 5.0e-2			PRD4 + HV = #.947 RO2-R. + #.053 RO2-N. + #.348 R2O2. + CCO-O2. + #.348 HCHO + #.613 RCHO + #.334 ACET + #.492 XC
Trans-2-Hexene [LP]	6.34e-11	6.34e-11			T-2-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 RCHO + #.902 XC
	1.15e-16	1.15e-16			T-2-C6E + O3 = #.301 HO. + #.04 RO2-R. + #.001 RO2-N. + #.26 C-O2. + #.301 CO + #.07 CO2 + #.5 CCHO + #.54 RCHO + #.17 CCO-OH + #.46 RCO-OH + #.07 INERT + #1.025 XC
	3.70e-13	3.70e-13			T-2-C6E + NO3 = #.12 NO2 + #.659 RO2-R. + #.221 RO2-N. + #.807 R2O2. + #.12 CCHO + #.134 RCHO + #.652 RNO3 + #.12 XC + #.228 XN
	2.05e-11	2.05e-11			T-2-C6E + O3P = #.76 MEK + #.24 PROD2 + #1.52 XC
Trans-2-Hexene [AP]	6.34e-11	6.34e-11			T-2-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 CCHO + #.902 XC + #.902 PRD1
	1.15e-16	1.15e-16			T-2-C6E + O3 = #.301 HO. + #.04 RO2-R. + #.001 RO2-N. + #.26 C-O2. + #.301 CO + #.07 CO2 + #.5 CCHO + #.04 RCHO + #.17 CCO-OH + #.46 RCO-OH + #.07 INERT + #1.025 XC + #.5 PRD1
	3.70e-13	3.70e-13			T-2-C6E + NO3 = #.12 NO2 + #.659 RO2-R. + #.221 RO2-N. + #.807 R2O2. + #.12 CCHO + #.007 RCHO + #.652 RNO3 + #.12 XC + #.127 PRD2 + #.228 XN
	2.05e-11	2.05e-11			T-2-C6E + O3P = #.76 MEK + #1.52 XC + #.24 PRD3
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	2.33e-11	2.33e-11			PRD2 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	7.51e-12	7.51e-12			PRD3 + HO. = #.434 RO2-R. + #.106 RO2-N. + #.839 R2O2. + #.23 CCO-O2. + #.23 RCO-O2. + #.24 HCHO + #.253 CCHO + #.445 RCHO + #.245 MEK + #.044 PROD2 + #.891 XC
		PF=KETONE QY = 5.0e-2			PRD3 + HV = #.955 RO2-R. + #.045 RO2-N. + #.377 R2O2. + #.5 CCO-O2. + #.5 RCO-O2. + #.955 RCHO + #.366 XC
Trans-3-Hexene [LP]	6.34e-11	6.34e-11			T-3-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #1.805 RCHO
	1.70e-16	6.64e-15	2.17		T-3-C6E + O3 = #.113 HO. + #.113 RO2-R. + #.113 CO + #.113 CCHO + RCHO + #.887 RCO-OH + #-0 XC
	3.70e-13	3.70e-13			T-3-C6E + NO3 = #.284 NO2 + #.514 RO2-R. + #.202 RO2-N. + #.774 R2O2. + #.567 RCHO + #.514 RNO3 + #.202 XN
	2.05e-11	2.05e-11			T-3-C6E + O3P = #.76 MEK + #.24 PROD2 + #1.52 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Trans-3-Hexene [AP]	6.34e-11	6.34e-11			T-3-C6E + HO. = #.902 RO2-R. + #.098 RO2-N. + #1.805 RCHO
	1.70e-16	6.64e-15	2.17		T-3-C6E + O3 = #.113 HO. + #.113 RO2-R. + #.113 CO + #.113 CCHO + RCHO + #.887 RCO-OH + #-0 XC
	3.70e-13	3.70e-13			T-3-C6E + NO3 = #.284 NO2 + #.514 RO2-R. + #.202 RO2-N. + #.774 R2O2. + #.567 RCHO + #.514 RNO3 + #.202 XN
	2.05e-11	2.05e-11			T-3-C6E + O3P = #.76 MEK + #1.52 XC + #.24 PRD1
	5.92e-12	5.92e-12			PRD1 + HO. = #.445 RO2-R. + #.11 RO2-N. + #.663 R2O2. + #.445 RCO-O2. + #.141 HCHO + #.312 CCHO + #.24 RCHO + #.344 MEK + #1.142 XC
	PF=KETONE QY = 5.0e-2				PRD1 + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #-0.06 XC
2,3-Dimethyl-2-Hexene	1.03e-10	1.92e-11	-0.99		23M2-C5E + HO. = #.865 RO2-R. + #.135 RO2-N. + #.865 ACET + #.865 MEK + #.135 XC
	6.74e-16	6.74e-16			23M2-C5E + O3 = HO. + #.02 RO2-N. + #.98 R2O2. + #.918 CCO-O2. + #.062 RCO-O2. + #.562 HCHO + #.418 CCHO + #.5 ACET + #.5 MEK + #-0.039 XC
	5.72e-11	5.72e-11			23M2-C5E + NO3 = #.865 NO2 + #.135 RO2-N. + #.865 R2O2. + #.865 ACET + #.865 MEK + #.135 XC + #.135 XN
	4.95e-11	4.95e-11			23M2-C5E + O3P = MEK + #3 XC
Cis-3-Heptene [LP]	6.34e-11	6.34e-11			C-3-C7E + HO. = #.865 RO2-R. + #.135 RO2-N. + #1.73 RCHO + XC
	1.15e-16	1.15e-16			C-3-C7E + O3 = #.098 HO. + #.097 RO2-R. + #.001 RO2-N. + #.098 CO + #.057 CCHO + #1.04 RCHO + #.903 RCO-OH + #.955 XC
	3.70e-13	3.70e-13			C-3-C7E + NO3 = #.082 NO2 + #.632 RO2-R. + #.286 RO2-N. + #.787 R2O2. + #.163 RCHO + #.632 RNO3 + XC + #.286 XN
	2.05e-11	2.05e-11			C-3-C7E + O3P = PROD2 + XC
Cis-3-Heptene [AP]	6.34e-11	6.34e-11			C-3-C7E + HO. = #.865 RO2-R. + #.135 RO2-N. + #.865 RCHO + XC + #.865 PRD1
	1.15e-16	1.15e-16			C-3-C7E + O3 = #.098 HO. + #.097 RO2-R. + #.001 RO2-N. + #.098 CO + #.057 CCHO + #.54 RCHO + #.903 RCO-OH + #.955 XC + #.5 PRD1
	3.70e-13	3.70e-13			C-3-C7E + NO3 = #.082 NO2 + #.632 RO2-R. + #.286 RO2-N. + #.787 R2O2. + #.082 RCHO + #.632 RNO3 + XC + #.082 PRD1 + #.286 XN
	2.05e-11	2.05e-11			C-3-C7E + O3P = XC + PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	5.91e-12	5.91e-12			PRD2 + HO. = #.271 RO2-R. + #.251 RO2-N. + #1.812 R2O2. + #.478 RCO-O2. + #.023 CO2 + #.049 HCHO + #.225 CCHO + #.304 RCHO + #.033 MEK + #.163 PROD2 + #.218 HCOOH + #.157 RCO-OH + #-0.205 XC
	PF=KETONE QY = 4.8e-3				PRD2 + HV = #.955 RO2-R. + #.045 RO2-N. + #.377 R2O2. + RCO-O2. + #.955 RCHO + #-0.134 XC
Trans 4,4-dimethyl-2-Pentene [LP]	5.52e-11	1.03e-11	-0.99		T44M2C5E + HO. = #.516 RO2-R. + #.149 RO2-N. + #.684 R2O2. + #.335 TBU-O. + #.516 CCHO + #.865 RCHO + #1.475 XC
	1.15e-16	1.15e-16			T44M2C5E + O3 = #.285 HO. + #.001 RO2-N. + #.024 R2O2. + #.26 C-O2. + #.024 TBU-O. + #.285 CO + #.07 CO2 + #.5 CCHO + #.5 RCHO + #.17 CCO-OH + #.475 RCO-OH + #.07 INERT + #2.042 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.70e-13	3.70e-13			T44M2C5E + NO3 = #.163 NO2 + #.205 RO2-R. + #.243 RO2-N. + #1.234 R2O2. + #.389 TBU-O. + #.026 HCHO + #.142 CCHO + #.569 RCHO + #.022 ACET + #.204 RNO3 + #1.07 XC + #.633 XN
	1.55e-11	1.55e-11			T44M2C5E + O3P = MEK + #3 XC
Trans 4,4-dimethyl-2-Pentene [AP]	5.52e-11	1.03e-11	-0.99		T44M2C5E + HO. = #.516 RO2-R. + #.149 RO2-N. + #.684 R2O2. + #.335 TBU-O. + #.516 CCHO + #1.475 XC + #.865 PRD1
	1.15e-16	1.15e-16			T44M2C5E + O3 = #.285 HO. + #.001 RO2-N. + #.024 R2O2. + #.26 C-O2. + #.024 TBU-O. + #.285 CO + #.07 CO2 + #.5 CCHO + #.17 CCO-OH + #.475 RCO-OH + #.07 INERT + #2.042 XC + #.5 PRD2
	3.70e-13	3.70e-13			T44M2C5E + NO3 = #.163 NO2 + #.205 RO2-R. + #.243 RO2-N. + #1.234 R2O2. + #.389 TBU-O. + #.026 HCHO + #.142 CCHO + #.022 ACET + #.204 RNO3 + #1.07 XC + #.569 PRD3 + #.633 XN
	1.55e-11	1.55e-11			T44M2C5E + O3P = MEK + #3 XC
	2.56e-11	2.56e-11			PRD1 + HO. = #.084 HO2. + #.014 RO2-R. + #.002 RO2-N. + #.014 R2O2. + #.9 RCO-O2. + #.014 CO + #.014 HCHO + #.014 ACET + #.084 MGLY + #-0.032 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.83 HO2. + #.573 RO2-R. + #.024 RO2-N. + #.573 TBU-O. + CO + #.403 CCHO + #-0.667 XC
	2.63e-11	2.63e-11			PRD2 + HO. = #.023 RO2-R. + #.003 RO2-N. + #.024 R2O2. + #.974 RCO-O2. + #.023 CO + #.024 HCHO + #.001 RCHO + #.023 ACET + #-0.054 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 TBU-O. + CO + #-1.118 XC
	2.12e-11	2.12e-11			PRD3 + HO. = #.006 RO2-R. + #.001 RO2-N. + #.006 R2O2. + #.993 RCO-O2. + #.006 CO + #.006 HCHO + #.006 ACET + #-0.014 XC + #.741 XN
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + #1.741 XN
		PF=C2CHO			PRD3 + HV = #.741 NO2 + #.751 HO2. + #.249 RO2-R. + #.01 RO2-N. + #.249 TBU-O. + CO + #.741 CCHO + #-0.29 XC
Trans-2-Heptene [LP]	6.80e-11	1.27e-11	-0.99		T-2-C7E + HO. = #.864 RO2-R. + #.136 RO2-N. + #.005 R2O2. + #.859 CCHO + #.859 RCHO + #.005 PROD2 + #1.859 XC
	1.15e-16	1.15e-16			T-2-C7E + O3 = #.285 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.26 C-O2. + #.285 CO + #.07 CO2 + #.5 CCHO + #.523 RCHO + #.475 PROD2 + #.17 CCO-OH + #.07 INERT + #.615 XC
	3.70e-13	3.70e-13			T-2-C7E + NO3 = #.013 NO2 + #.689 RO2-R. + #.299 RO2-N. + #.809 R2O2. + #.013 CCHO + #.013 RCHO + #.689 RNO3 + #1.013 XC + #.299 XN
	2.29e-11	2.29e-11			T-2-C7E + O3P = PROD2 + XC
Trans-2-Heptene [AP]	6.80e-11	1.27e-11	-0.99		T-2-C7E + HO. = #.864 RO2-R. + #.136 RO2-N. + #.005 R2O2. + #.859 CCHO + #.005 PROD2 + #1.859 XC + #.859 PRD1
	1.15e-16	1.15e-16			T-2-C7E + O3 = #.285 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.26 C-O2. + #.285 CO + #.07 CO2 + #.5 CCHO + #.17 CCO-OH + #.07 INERT + #.615 XC + #.523 PRD2 + #.475 PRD3
	3.70e-13	3.70e-13			T-2-C7E + NO3 = #.013 NO2 + #.689 RO2-R. + #.299 RO2-N. + #.809 R2O2. + #.013 CCHO + #.689 RNO3 + #1.013 XC + #.013 PRD1 + #.299 XN
	2.29e-11	2.29e-11			T-2-C7E + O3P = XC + PRD4
	2.82e-11	2.82e-11			PRD1 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.82e-11	2.82e-11			PRD2 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC
	6.76e-12	6.76e-12			PRD3 + HO. = #.926 RO2-R. + #.074 RO2-N. + #.549 R2O2. + #.016 CO2 + #.327 CCHO + #.434 RCHO + #.091 PROD2 + #.07 MGLY + #.111 BACL + #.29 RCO-OH + #1.513 XC
	6.32e-12	6.32e-12			PRD4 + HO. = #.315 RO2-R. + #.269 RO2-N. + #1.878 R2O2. + #.363 CCO-O2. + #.053 RCO-O2. + #.014 CO2 + #.036 HCHO + #.142 CCHO + #.428 RCHO + #.025 MEK + #.27 PROD2 + #.176 HCOOH + #.01 CCO-OH + #-0.051 XC
		PF=KETONE QY = 4.8e-3			PRD4 + HV = #.903 RO2-R. + #.097 RO2-N. + #.845 R2O2. + #.5 CCO-O2. + #.5 RCO-O2. + #.903 RCHO + #.208 XC
Trans-3-Heptene [LP]	6.34e-11	6.34e-11			T-3-C7E + HO. = #.865 RO2-R. + #.135 RO2-N. + #1.73 RCHO + XC
	1.15e-16	1.15e-16			T-3-C7E + O3 = #.098 HO. + #.097 RO2-R. + #.001 RO2-N. + #.098 CO + #.057 CCHO + #1.04 RCHO + #.903 RCO-OH + #.955 XC
	3.70e-13	3.70e-13			T-3-C7E + NO3 = #.082 NO2 + #.632 RO2-R. + #.286 RO2-N. + #.787 R2O2. + #.163 RCHO + #.632 RNO3 + XC + #.286 XN
	2.05e-11	2.05e-11			T-3-C7E + O3P = PROD2 + XC
Trans-3-Heptene [AP]	6.34e-11	6.34e-11			T-3-C7E + HO. = #.865 RO2-R. + #.135 RO2-N. + #.865 RCHO + XC + #.865 PRD1
	1.15e-16	1.15e-16			T-3-C7E + O3 = #.098 HO. + #.097 RO2-R. + #.001 RO2-N. + #.098 CO + #.057 CCHO + #.54 RCHO + #.903 RCO-OH + #.955 XC + #.5 PRD1
	3.70e-13	3.70e-13			T-3-C7E + NO3 = #.082 NO2 + #.632 RO2-R. + #.286 RO2-N. + #.787 R2O2. + #.082 RCHO + #.632 RNO3 + XC + #.082 PRD1 + #.286 XN
	2.05e-11	2.05e-11			T-3-C7E + O3P = XC + PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	5.91e-12	5.91e-12			PRD2 + HO. = #.271 RO2-R. + #.251 RO2-N. + #1.812 R2O2. + #.478 RCO-O2. + #.023 CO2 + #.049 HCHO + #.225 CCHO + #.304 RCHO + #.033 MEK + #.163 PROD2 + #.218 HCOOH + #.157 RCO-OH + #-0.205 XC
		PF=KETONE QY = 4.8e-3			PRD2 + HV = #.955 RO2-R. + #.045 RO2-N. + #.377 R2O2. + RCO-O2. + #.955 RCHO + #-0.134 XC
Cis-4-Octene [LP]	6.34e-11	6.34e-11			C-4-C8E + HO. = #.827 RO2-R. + #.173 RO2-N. + #1.653 RCHO + #2 XC
	9.51e-17	3.22e-15	2.09		C-4-C8E + O3 = #.082 HO. + #.08 RO2-R. + #.002 RO2-N. + #.082 CO + #1.08 RCHO + #.919 RCO-OH + #1.91 XC
	3.70e-13	3.70e-13			C-4-C8E + NO3 = #.014 NO2 + #.634 RO2-R. + #.352 RO2-N. + #.781 R2O2. + #.028 RCHO + #.634 RNO3 + #2 XC + #.352 XN
	2.05e-11	2.05e-11			C-4-C8E + O3P = PROD2 + #2 XC
Cis-4-Octene [AP]	6.34e-11	6.34e-11			C-4-C8E + HO. = #.827 RO2-R. + #.173 RO2-N. + #2 XC + #1.653 PRD1
	9.51e-17	3.22e-15	2.09		C-4-C8E + O3 = #.082 HO. + #.08 RO2-R. + #.002 RO2-N. + #.082 CO + #.08 RCHO + #.919 RCO-OH + #1.91 XC + PRD1
	3.70e-13	3.70e-13			C-4-C8E + NO3 = #.014 NO2 + #.634 RO2-R. + #.352 RO2-N. + #.781 R2O2. + #.634 RNO3 + #2 XC + #.028 PRD1 + #.352 XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.05e-11	2.05e-11			C-4-C8E + O3P = #2 XC + PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	7.63e-12	7.63e-12			PRD2 + HO. = #.307 RO2-R. + #.334 RO2-N. + #1.717 R2O2. + #.358 RCO-O2. + #.013 CO2 + #.049 HCHO + #.069 CCHO + #.392 RCHO + #.028 MEK + #.234 PROD2 + #.141 HCOOH + #.128 RCO-OH + #-0.505 XC
		PF=KETONE QY = 2.4e-3			PRD2 + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #-0.06 XC
Trans 2,2-Dimethyl 3-Hexene [LP]	6.34e-11	6.34e-11			T22M3C6E + HO. = #.432 RO2-R. + #.189 RO2-N. + #.773 R2O2. + #.379 TBU-O. + #1.259 RCHO + #1.953 XC
	4.20e-17	6.64e-15	3.00		T22M3C6E + O3 = #.082 HO. + #.057 RO2-R. + #.001 RO2-N. + #.024 R2O2. + #.024 TBU-O. + #.082 CO + #.057 CCHO + RCHO + #.918 RCO-OH + #1.972 XC
	3.70e-13	3.70e-13			T22M3C6E + NO3 = #.154 NO2 + #.193 RO2-R. + #.278 RO2-N. + #1.175 R2O2. + #.375 TBU-O. + #.017 HCHO + #.011 CCHO + #.706 RCHO + #.002 ACET + #.183 RNO3 + #1.948 XC + #.664 XN
	2.05e-11	2.05e-11			T22M3C6E + O3P = #.88 MEK + #.12 PROD2 + #3.76 XC
Trans 2,2-Dimethyl 3-Hexene [AP]	6.34e-11	6.34e-11			T22M3C6E + HO. = #.432 RO2-R. + #.189 RO2-N. + #.773 R2O2. + #.379 TBU-O. + #.432 RCHO + #1.953 XC + #.827 PRD1
	4.20e-17	6.64e-15	3.00		T22M3C6E + O3 = #.082 HO. + #.057 RO2-R. + #.001 RO2-N. + #.024 R2O2. + #.024 TBU-O. + #.082 CO + #.057 CCHO + #.5 RCHO + #.918 RCO-OH + #1.972 XC + #.5 PRD2
	3.70e-13	3.70e-13			T22M3C6E + NO3 = #.154 NO2 + #.193 RO2-R. + #.278 RO2-N. + #1.175 R2O2. + #.375 TBU-O. + #.017 HCHO + #.011 CCHO + #.152 RCHO + #.002 ACET + #.183 RNO3 + #1.948 XC + #.555 PRD3 + #.664 XN
	2.05e-11	2.05e-11			T22M3C6E + O3P = #.88 MEK + #3.76 XC + #.12 PRD4
	2.66e-11	2.66e-11			PRD1 + HO. = #.112 HO2. + #.032 RO2-R. + #.002 RO2-N. + #.012 R2O2. + #.854 RCO-O2. + #.012 CO + #.012 HCHO + #.02 CCHO + #.012 ACET + #.02 GLY + #.112 MGLY + #-0.051 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.975 HO2. + #.502 RO2-R. + #.021 RO2-N. + #.502 TBU-O. + CO + #.477 RCHO + #-1.062 XC
	2.63e-11	2.63e-11			PRD2 + HO. = #.023 RO2-R. + #.003 RO2-N. + #.024 R2O2. + #.974 RCO-O2. + #.023 CO + #.024 HCHO + #.001 RCHO + #.023 ACET + #-0.054 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 TBU-O. + CO + #-1.118 XC
	2.22e-11	2.22e-11			PRD3 + HO. = #.019 NO2 + #.025 RO2-R. + #.004 RO2-N. + #.026 R2O2. + #.952 RCO-O2. + #.006 CO + #.007 HCHO + #.019 CCHO + #.019 RCHO + #.006 ACET + #.019 GLY + #-0.044 XC + #.701 XN
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + #-0 XC + #1.72 XN
		PF=C2CHO			PRD3 + HV = #.72 NO2 + #.731 HO2. + #.269 RO2-R. + #.011 RO2-N. + #.269 TBU-O. + CO + #.72 RCHO + #-1.033 XC
	6.29e-12	6.29e-12			PRD4 + HO. = #.363 RO2-R. + #.215 RO2-N. + #.771 R2O2. + #.422 RCO-O2. + #.336 HCHO + #.143 CCHO + #.142 RCHO + #.179 ACET + #.335 MEK + #.519 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=KETONE QY = 1.0e-2				PRD4 + HV = #.039 RO2-N. + #.961 R2O2. + RCO-O2. + #.961 TBU-O. + #-0.118 XC
Trans 2,5-Dimethyl 3-Hexene [LP]	6.34e-11	6.34e-11			T25M3C6E + HO. = #.827 RO2-R. + #.173 RO2-N. + #1.653 RCHO + #2 XC
	4.10e-17	6.64e-15	3.01		T25M3C6E + O3 = #.082 HO. + #.079 RO2-R. + #.003 RO2-N. + #.082 CO + RCHO + #.079 ACET + #.919 RCO-OH + #1.905 XC
	3.70e-13	3.70e-13			T25M3C6E + NO3 = #.168 NO2 + #.55 RO2-R. + #.282 RO2-N. + #.762 R2O2. + #.636 RCHO + #.288 ACET + #.262 RNO3 + #1.964 XC + #.57 XN
	2.05e-11	2.05e-11			T25M3C6E + O3P = PROD2 + #2 XC
Trans 2,5-Dimethyl 3-Hexene [AP]	6.34e-11	6.34e-11			T25M3C6E + HO. = #.827 RO2-R. + #.173 RO2-N. + #2 XC + #1.653 PRD1
	4.10e-17	6.64e-15	3.01		T25M3C6E + O3 = #.082 HO. + #.079 RO2-R. + #.003 RO2-N. + #.082 CO + #.079 ACET + #.919 RCO-OH + #1.905 XC + PRD1
	3.70e-13	3.70e-13			T25M3C6E + NO3 = #.168 NO2 + #.55 RO2-R. + #.282 RO2-N. + #.762 R2O2. + #.288 ACET + #.262 RNO3 + #1.964 XC + #.636 PRD2 + #.57 XN
	2.05e-11	2.05e-11			T25M3C6E + O3P = #2 XC + PRD3
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	2.41e-11	2.41e-11			PRD2 + HO. = #.047 NO2 + #.043 RO2-R. + #.006 RO2-N. + #.061 R2O2. + #.001 C-O2. + #.903 RCO-O2. + #.041 CO + #.006 HCHO + #.006 CCHO + #.003 RCHO + #.083 ACET + #.047 GLY + #-0.154 XC + #.425 XN
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #1.472 XN
		PF=C2CHO			PRD2 + HV = #.472 NO2 + HO2. + #.507 RO2-R. + #.021 RO2-N. + CO + #.472 RCHO + #.507 ACET + #-1.063 XC
	7.58e-12	7.58e-12			PRD3 + HO. = #.19 RO2-R. + #.288 RO2-N. + #1.948 R2O2. + #.003 C-O2. + #.519 RCO-O2. + #.019 CO2 + #.173 HCHO + #.056 CCHO + #.041 RCHO + #.728 ACET + #.124 MEK + #.329 HCOOH + #.015 RCO-OH + #-0.82 XC
	PF=KETONE QY = 2.4e-3				PRD3 + HV = #.947 RO2-R. + #.053 RO2-N. + #.348 R2O2. + RCO-O2. + #.348 HCHO + #.613 RCHO + #.334 ACET + #-0.508 XC
Trans-3-Octene [LP]	6.34e-11	6.34e-11			T-3-C8E + HO. = #.826 RO2-R. + #.174 RO2-N. + #.004 R2O2. + #1.644 RCHO + #.004 PROD2 + #2 XC
	1.15e-16	1.15e-16			T-3-C8E + O3 = #.082 HO. + #.08 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.082 CO + #.057 CCHO + #1.023 RCHO + #.475 PROD2 + #.444 RCO-OH + #.545 XC
	3.70e-13	3.70e-13			T-3-C8E + NO3 = #.014 NO2 + #.634 RO2-R. + #.352 RO2-N. + #.781 R2O2. + #.027 RCHO + #.634 RNO3 + #2 XC + #.352 XN
	2.05e-11	2.05e-11			T-3-C8E + O3P = PROD2 + #2 XC
Trans-3-Octene [AP]	6.34e-11	6.34e-11			T-3-C8E + HO. = #.826 RO2-R. + #.174 RO2-N. + #.004 R2O2. + #.822 RCHO + #.004 PROD2 + #2 XC + #.822 PRD1
	1.15e-16	1.15e-16			T-3-C8E + O3 = #.082 HO. + #.08 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.082 CO + #.057 CCHO + #.5 RCHO + #.444 RCO-OH + #.545 XC + #.523 PRD2 + #.475 PRD3
	3.70e-13	3.70e-13			T-3-C8E + NO3 = #.014 NO2 + #.634 RO2-R. + #.352 RO2-N. + #.781 R2O2. + #.014 RCHO + #.634 RNO3 + #2 XC + #.014 PRD1 + #.352 XN
	2.05e-11	2.05e-11			T-3-C8E + O3P = #2 XC + PRD4

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.82e-11	2.82e-11			PRD1 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC
	2.82e-11	2.82e-11			PRD2 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC
	6.76e-12	6.76e-12			PRD3 + HO. = #.926 RO2-R. + #.074 RO2-N. + #.549 R2O2. + #.016 CO2 + #.327 CCHO + #.434 RCHO + #.091 PROD2 + #.07 MGLY + #.111 BACL + #.29 RCO-OH + #1.513 XC
	7.39e-12	7.39e-12			PRD4 + HO. = #.335 RO2-R. + #.352 RO2-N. + #1.731 R2O2. + #.312 RCO-O2. + #.012 CO2 + #.02 HCHO + #.209 CCHO + #.33 RCHO + #.004 MEK + #.322 PROD2 + #.119 HCOOH + #.008 RCO-OH + #-0.594 XC
		PF=KETONE QY = 2.4e-3			PRD4 + HV = #.927 RO2-R. + #.073 RO2-N. + #.468 R2O2. + RCO-O2. + #.927 RCHO + #-0.218 XC
Trans-4-Octene [LP]	6.91e-11	1.29e-11	-0.99		T-4-C8E + HO. = #.827 RO2-R. + #.173 RO2-N. + #1.653 RCHO + #2 XC
	1.40e-16	6.64e-15	2.29		T-4-C8E + O3 = #.082 HO. + #.08 RO2-R. + #.002 RO2-N. + #.082 CO + #1.08 RCHO + #.919 RCO-OH + #1.91 XC
	3.70e-13	3.70e-13			T-4-C8E + NO3 = #.014 NO2 + #.634 RO2-R. + #.352 RO2-N. + #.781 R2O2. + #.028 RCHO + #.634 RNO3 + #2 XC + #.352 XN
	2.36e-11	2.36e-11			T-4-C8E + O3P = PROD2 + #2 XC
Trans-4-Octene [AP]	6.91e-11	1.29e-11	-0.99		T-4-C8E + HO. = #.827 RO2-R. + #.173 RO2-N. + #2 XC + #1.653 PRD1
	1.40e-16	6.64e-15	2.29		T-4-C8E + O3 = #.082 HO. + #.08 RO2-R. + #.002 RO2-N. + #.082 CO + #.08 RCHO + #.919 RCO-OH + #1.91 XC + PRD1
	3.70e-13	3.70e-13			T-4-C8E + NO3 = #.014 NO2 + #.634 RO2-R. + #.352 RO2-N. + #.781 R2O2. + #.634 RNO3 + #2 XC + #.028 PRD1 + #.352 XN
	2.36e-11	2.36e-11			T-4-C8E + O3P = #2 XC + PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	7.63e-12	7.63e-12			PRD2 + HO. = #.307 RO2-R. + #.334 RO2-N. + #1.717 R2O2. + #.358 RCO-O2. + #.013 CO2 + #.049 HCHO + #.069 CCHO + #.392 RCHO + #.028 MEK + #.234 PROD2 + #.141 HCOOH + #.128 RCO-OH + #-0.505 XC
		PF=KETONE QY = 2.4e-3			PRD2 + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #-0.06 XC
2,4,4-trimethyl-2-Pentene [LP]	8.71e-11	8.71e-11			244M2C5E + HO. = #.784 RO2-R. + #.216 RO2-N. + #.056 R2O2. + #.025 CCHO + #.784 RCHO + #.784 ACET + #2.95 XC
	1.40e-16	2.87e-15	1.79		244M2C5E + O3 = #.7 HO. + #.7 R2O2. + #.7 CCO-O2. + #.7 HCHO + #.7 RCHO + #.3 ACET + #.3 RCO-OH + #3 XC
	9.37e-12	9.37e-12			244M2C5E + NO3 = #.524 NO2 + #.036 RO2-R. + #.44 RO2-N. + #1.86 R2O2. + #.077 HCHO + #.53 CCHO + #.525 RCHO + #.492 ACET + #.032 MEK + #.035 RNO3 + #1.832 XC + #.441 XN
	3.71e-11	3.71e-11			244M2C5E + O3P = #.6 MEK + #.4 PROD2 + #4.2 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
2,4,4-trimethyl-2-Pentene [AP]	8.71e-11	8.71e-11			244M2C5E + HO. = #.784 RO2-R. + #.216 RO2-N. + #.056 R2O2. + #.025 CCHO + #.784 ACET + #2.95 XC + #.784 PRD1
	1.40e-16	2.87e-15	1.79		244M2C5E + O3 = #.7 HO. + #.7 R2O2. + #.7 CCO-O2. + #.7 HCHO + #.3 ACET + #.3 RCO-OH + #3 XC + #.7 PRD2
	9.37e-12	9.37e-12			244M2C5E + NO3 = #.524 NO2 + #.036 RO2-R. + #.44 RO2-N. + #1.86 R2O2. + #.077 HCHO + #.53 CCHO + #.492 ACET + #.032 MEK + #.035 RNO3 + #1.832 XC + #.525 PRD3 + #.441 XN
	3.71e-11	3.71e-11			244M2C5E + O3P = #.6 MEK + #4.2 XC + #.4 PRD4
	2.09e-11	2.09e-11			PRD1 + HO. = #.059 RO2-R. + #.013 RO2-N. + #.062 R2O2. + #.928 RCO-O2. + #.058 CO + #.014 HCHO + #.047 CCHO + #.001 RCHO + #.045 ACET + #.013 MEK + #-0.219 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.052 HO2. + #1.856 RO2-R. + #.052 RO2-N. + #.04 C-O2. + CO + #.908 CCHO + #.908 ACET + #.04 MEK + #-3.052 XC
	2.09e-11	2.09e-11			PRD2 + HO. = #.059 RO2-R. + #.013 RO2-N. + #.062 R2O2. + #.928 RCO-O2. + #.058 CO + #.014 HCHO + #.047 CCHO + #.001 RCHO + #.045 ACET + #.013 MEK + #-0.219 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.052 HO2. + #1.856 RO2-R. + #.052 RO2-N. + #.04 C-O2. + CO + #.908 CCHO + #.908 ACET + #.04 MEK + #-3.052 XC
	1.99e-11	1.99e-11			PRD3 + HO. = #.023 RO2-R. + #.002 RO2-N. + #.008 R2O2. + #.975 RCO-O2. + #.008 CO + #.016 HCHO + #.006 CCHO + #.006 ACET + #.002 MEK + #.014 MGLY + #-0.046 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #1.735 HO2. + #.253 RO2-R. + #.007 RO2-N. + #.005 C-O2. + CO + #.124 CCHO + #.987 ACET + #.005 MEK + #-1.28 XC
	7.42e-12	7.42e-12			PRD4 + HO. = #.05 RO2-R. + #.297 RO2-N. + #1.258 R2O2. + #.653 RCO-O2. + #.193 HCHO + #.459 CCHO + #.05 RCHO + #.493 ACET + #.089 MEK + #.001 PROD2 + #-0.844 XC
Trans-4-Nonene [LP]	6.34e-11	6.34e-11			T-4-C9E + HO. = #.793 RO2-R. + #.207 RO2-N. + #.005 R2O2. + #1.577 RCHO + #.004 PROD2 + #3 XC
	1.15e-16	1.15e-16			T-4-C9E + O3 = #.066 HO. + #.063 RO2-R. + #.003 RO2-N. + #.019 R2O2. + #.066 CO + #1.063 RCHO + #.475 PROD2 + #.46 RCO-OH + #1.5 XC
	3.70e-13	3.70e-13			T-4-C9E + NO3 = #.005 NO2 + #.6 RO2-R. + #.395 RO2-N. + #.761 R2O2. + #.01 RCHO + #.6 RNO3 + #3 XC + #.395 XN
	2.05e-11	2.05e-11			T-4-C9E + O3P = PROD2 + #3 XC
Trans-4-Nonene [AP]	6.34e-11	6.34e-11			T-4-C9E + HO. = #.793 RO2-R. + #.207 RO2-N. + #.005 R2O2. + #.004 PROD2 + #3 XC + #1.577 PRD1
	1.15e-16	1.15e-16			T-4-C9E + O3 = #.066 HO. + #.063 RO2-R. + #.003 RO2-N. + #.019 R2O2. + #.066 CO + #.04 RCHO + #.46 RCO-OH + #1.5 XC + #1.023 PRD2 + #.475 PRD3
	3.70e-13	3.70e-13			T-4-C9E + NO3 = #.005 NO2 + #.6 RO2-R. + #.395 RO2-N. + #.761 R2O2. + #.01 RCHO + #.6 RNO3 + #3 XC + #.395 XN
	2.05e-11	2.05e-11			T-4-C9E + O3P = #3 XC + PRD4
	2.57e-11	2.57e-11			PRD1 + HO. = #.088 RO2-R. + #.013 RO2-N. + #.047 R2O2. + #.899 RCO-O2. + #.047 CO + #.013 HCHO + #.018 CCHO + #.08 RCHO + #.001 GLY + #.001 MGLY + #-0.112 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.623 HO2. + #1.333 RO2-R. + #.045 RO2-N. + CO + #.955 RCHO + #-1.134 XC
	2.57e-11	2.57e-11			PRD2 + HO. = #.088 RO2-R. + #.013 RO2-N. + #.047 R2O2. + #.899 RCO-O2. + #.047 CO + #.013 HCHO + #.018 CCHO + #.08 RCHO + #.001 GLY + #.001 MGLY + #-0.112 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD2 + HV = #.624 HO2. + #1.331 RO2-R. + #.044 RO2-N. + CO + #.956 RCHO + #-1.133 XC
	6.76e-12	6.76e-12			PRD3 + HO. = #.926 RO2-R. + #.074 RO2-N. + #.549 R2O2. + #.016 CO2 + #.327 CCHO + #.434 RCHO + #.091 PROD2 + #.07 MGLY + #.111 BACL + #.29 RCO-OH + #1.513 XC
	9.12e-12	9.12e-12			PRD4 + HO. = #.362 RO2-R. + #.424 RO2-N. + #1.635 R2O2. + #.214 RCO-O2. + #.005 CO2 + #.027 HCHO + #.083 CCHO + #.383 RCHO + #.012 MEK + #.337 PROD2 + #.065 HCOOH + #.006 RCO-OH + #-0.689 XC
3,4-Diethyl-2-Hexene [LP]	8.71e-11	8.71e-11			34E2-C6E + HO. = #.77 RO2-R. + #.23 RO2-N. + #.77 CCHO + #.77 PROD2 + #2.46 XC
	4.21e-18	2.87e-15	3.86		34E2-C6E + O3 = #.856 HO. + #.121 RO2-N. + #.579 R2O2. + #.156 C-O2. + #.579 RCO-O2. + #.156 CO + #.042 CO2 + #.841 CCHO + #.438 MEK + #.3 PROD2 + #.102 CCO-OH + #.042 INERT + #1.745 XC
	9.37e-12	9.37e-12			34E2-C6E + NO3 = #.048 NO2 + #.629 RO2-R. + #.323 RO2-N. + #1.057 R2O2. + #.314 CCHO + #.274 RCHO + #.354 MEK + #.048 PROD2 + #.699 RNO3 + #.717 XC + #.253 XN
	3.71e-11	3.71e-11			34E2-C6E + O3P = PROD2 + #4 XC
3,4-Diethyl-2-Hexene [AP]	8.71e-11	8.71e-11			34E2-C6E + HO. = #.77 RO2-R. + #.23 RO2-N. + #.77 CCHO + #2.46 XC + #.77 PRD1
	4.21e-18	2.87e-15	3.86		34E2-C6E + O3 = #.856 HO. + #.121 RO2-N. + #.579 R2O2. + #.156 C-O2. + #.579 RCO-O2. + #.156 CO + #.042 CO2 + #.841 CCHO + #.438 MEK + #.102 CCO-OH + #.042 INERT + #1.745 XC + #.3 PRD1
	9.37e-12	9.37e-12			34E2-C6E + NO3 = #.048 NO2 + #.629 RO2-R. + #.323 RO2-N. + #1.057 R2O2. + #.314 CCHO + #.274 RCHO + #.354 MEK + #.699 RNO3 + #.717 XC + #.048 PRD1 + #.253 XN
	3.71e-11	3.71e-11			34E2-C6E + O3P = #4 XC + PRD2
	1.11e-11	1.11e-11			PRD1 + HO. = #.052 RO2-R. + #.234 RO2-N. + #1.298 R2O2. + #.714 RCO-O2. + #.595 CCHO + #.535 RCHO + #.172 MEK + #.006 PROD2 + #-1.065 XC
		PF=KETONE QY = 1.0e-2			PRD1 + HV = #.884 RO2-R. + #.116 RO2-N. + #.375 R2O2. + RCO-O2. + #.375 CCHO + #.375 RCHO + #.509 MEK + #-1.607 XC
	1.29e-11	1.29e-11			PRD2 + HO. = #.133 RO2-R. + #.393 RO2-N. + #1.737 R2O2. + #.474 CCO-O2. + #.006 HCHO + #.221 CCHO + #.315 RCHO + #.507 MEK + #.102 PROD2 + #.176 RCO-OH + #-1.873 XC
Cis-5-Decene [LP]	6.34e-11	6.34e-11			C-5-C10E + HO. = #.768 RO2-R. + #.232 RO2-N. + #.01 R2O2. + #1.519 RCHO + #.008 PROD2 + #4 XC
	1.20e-16	3.22e-15	1.95		C-5-C10E + O3 = #.05 HO. + #.047 RO2-R. + #.003 RO2-N. + #.038 R2O2. + #.05 CO + #1.047 RCHO + #.95 PROD2 + #1.09 XC
	3.70e-13	3.70e-13			C-5-C10E + NO3 = #.577 RO2-R. + #.423 RO2-N. + #.749 R2O2. + #.577 RNO3 + #4 XC + #.423 XN
	2.05e-11	2.05e-11			C-5-C10E + O3P = PROD2 + #4 XC
Cis-5-Decene [AP]	6.34e-11	6.34e-11			C-5-C10E + HO. = #.768 RO2-R. + #.232 RO2-N. + #.01 R2O2. + #.008 PROD2 + #4 XC + #1.519 PRD1
	1.20e-16	3.22e-15	1.95		C-5-C10E + O3 = #.05 HO. + #.047 RO2-R. + #.003 RO2-N. + #.038 R2O2. + #.05 CO + #1.09 XC + #1.047 PRD2 + #.95 PRD3
	3.70e-13	3.70e-13			C-5-C10E + NO3 = #.577 RO2-R. + #.423 RO2-N. + #.749 R2O2. + #.577 RNO3 + #4 XC + #.423 XN
	2.05e-11	2.05e-11			C-5-C10E + O3P = #4 XC + PRD4
	2.82e-11	2.82e-11			PRD1 + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #-0.149 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #-1.208 XC
	2.81e-11	2.81e-11			PRD2 + HO. = #.006 HO2. + #.089 RO2-R. + #.017 RO2-N. + #.077 R2O2. + #.888 RCO-O2. + #.042 CO + #.013 HCHO + #.02 CCHO + #.092 RCHO + #.002 MGLY + #-0.147 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.271 HO2. + #1.662 RO2-R. + #.067 RO2-N. + CO + #.001 HCHO + #.933 RCHO + #-1.2 XC
	6.76e-12	6.76e-12			PRD3 + HO. = #.926 RO2-R. + #.074 RO2-N. + #.549 R2O2. + #.016 CO2 + #.327 CCHO + #.434 RCHO + #.091 PROD2 + #.07 MGLY + #.111 BACL + #.29 RCO-OH + #1.513 XC
	1.06e-11	1.06e-11			PRD4 + HO. = #.421 RO2-R. + #.5 RO2-N. + #1.572 R2O2. + #.079 RCO-O2. + #.013 HCHO + #.087 CCHO + #.367 RCHO + #.001 MEK + #.324 PROD2 + #.011 HCOOH + #-0.488 XC
Trans-4-Decene [LP]	6.34e-11	6.34e-11			T-4-C10E + HO. = #.768 RO2-R. + #.232 RO2-N. + #.01 R2O2. + #1.519 RCHO + #.008 PROD2 + #4 XC
	1.15e-16	1.15e-16			T-4-C10E + O3 = #.041 HO. + #.04 RO2-R. + #.001 RO2-N. + #.041 CO + #1.04 RCHO + #.5 PROD2 + #.46 RCO-OH + #2.455 XC
	3.70e-13	3.70e-13			T-4-C10E + NO3 = #.005 NO2 + #.573 RO2-R. + #.422 RO2-N. + #.749 R2O2. + #.01 RCHO + #.573 RNO3 + #4 XC + #.422 XN
	2.05e-11	2.05e-11			T-4-C10E + O3P = PROD2 + #4 XC
Trans-4-Decene [AP]	6.34e-11	6.34e-11			T-4-C10E + HO. = #.768 RO2-R. + #.232 RO2-N. + #.01 R2O2. + #.008 PROD2 + #4 XC + #1.519 PRD1
	1.15e-16	1.15e-16			T-4-C10E + O3 = #.041 HO. + #.04 RO2-R. + #.001 RO2-N. + #.041 CO + #.04 RCHO + #.46 RCO-OH + #2.455 XC + PRD2 + #.5 PRD3
	3.70e-13	3.70e-13			T-4-C10E + NO3 = #.005 NO2 + #.573 RO2-R. + #.422 RO2-N. + #.749 R2O2. + #.01 RCHO + #.573 RNO3 + #4 XC + #.422 XN
	2.05e-11	2.05e-11			T-4-C10E + O3P = #4 XC + PRD4
	2.38e-11	2.38e-11			PRD1 + HO. = #.1 RO2-R. + #.024 RO2-N. + #.085 R2O2. + #.876 RCO-O2. + #.033 CO + #.008 HCHO + #.007 CCHO + #.088 RCHO + #.009 MGLY + #-0.121 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.532 HO2. + #1.395 RO2-R. + #.073 RO2-N. + CO + #.927 RCHO + #-1.218 XC
	2.38e-11	2.38e-11			PRD2 + HO. = #.1 RO2-R. + #.024 RO2-N. + #.085 R2O2. + #.876 RCO-O2. + #.033 CO + #.008 HCHO + #.007 CCHO + #.088 RCHO + #.009 MGLY + #-0.121 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.532 HO2. + #1.395 RO2-R. + #.073 RO2-N. + CO + #.927 RCHO + #-1.218 XC
	8.18e-12	8.18e-12			PRD3 + HO. = #.845 RO2-R. + #.155 RO2-N. + #.766 R2O2. + #.013 CO2 + #.014 CCHO + #.38 RCHO + #.544 PROD2 + #.012 MGLY + #.085 BACL + #.251 XC
	1.05e-11	1.05e-11			PRD4 + HO. = #.338 RO2-R. + #.475 RO2-N. + #1.55 R2O2. + #.187 RCO-O2. + #.005 CO2 + #.017 HCHO + #.024 CCHO + #.365 RCHO + #.009 MEK + #.327 PROD2 + #.063 HCOOH + #.004 RCO-OH + #-0.656 XC
Trans-5-Undecene [LP]	6.34e-11	6.34e-11			T-5-C11E + HO. = #.751 RO2-R. + #.249 RO2-N. + #.015 R2O2. + #1.479 RCHO + #.011 PROD2 + #5 XC
	1.15e-16	1.15e-16			T-5-C11E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #1.023 RCHO + #.975 PROD2 + #2.045 XC
	3.70e-13	3.70e-13			T-5-C11E + NO3 = #.56 RO2-R. + #.44 RO2-N. + #.742 R2O2. + #.56 RNO3 + #5 XC + #.44 XN
	2.05e-11	2.05e-11			T-5-C11E + O3P = PROD2 + #5 XC
Trans-5-Undecene [AP]	6.34e-11	6.34e-11			T-5-C11E + HO. = #.751 RO2-R. + #.249 RO2-N. + #.015 R2O2. + #.011 PROD2 + #5 XC + #1.479 PRD1

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.15e-16	1.15e-16			T-5-C11E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #2.045 XC + #1.023 PRD2 + #.975 PRD3
	3.70e-13	3.70e-13			T-5-C11E + NO3 = #.56 RO2-R. + #.44 RO2-N. + #.742 R2O2. + #.56 RNO3 + #5 XC + #.44 XN
	2.05e-11	2.05e-11			T-5-C11E + O3P = #5 XC + PRD4
	2.62e-11	2.62e-11			PRD1 + HO. = #.1 RO2-R. + #.029 RO2-N. + #.117 R2O2. + #.87 RCO-O2. + #.028 CO + #.007 HCHO + #.01 CCHO + #.095 RCHO + #.01 MGLY + #-0.158 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.155 HO2. + #1.748 RO2-R. + #.097 RO2-N. + CO + #.903 RCHO + #-1.292 XC
	2.62e-11	2.62e-11			PRD2 + HO. = #.1 RO2-R. + #.029 RO2-N. + #.117 R2O2. + #.87 RCO-O2. + #.028 CO + #.007 HCHO + #.01 CCHO + #.095 RCHO + #.01 MGLY + #-0.158 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.155 HO2. + #1.748 RO2-R. + #.097 RO2-N. + CO + #.903 RCHO + #-1.292 XC
	7.49e-12	7.49e-12			PRD3 + HO. = #.884 RO2-R. + #.116 RO2-N. + #.66 R2O2. + #.014 CO2 + #.166 CCHO + #.406 RCHO + #.323 PROD2 + #.04 MGLY + #.098 BACL + #.141 RCO-OH + #.866 XC
	1.20e-11	1.20e-11			PRD4 + HO. = #.399 RO2-R. + #.536 RO2-N. + #1.513 R2O2. + #.066 RCO-O2. + #.007 HCHO + #.037 CCHO + #.351 RCHO + #.001 MEK + #.323 PROD2 + #.009 HCOOH + #-0.497 XC
Trans-5-Dodecene [LP]	6.34e-11	6.34e-11			T-5-C12E + HO. = #.741 RO2-R. + #.259 RO2-N. + #.015 R2O2. + #1.461 RCHO + #.011 PROD2 + #6 XC
	1.15e-16	1.15e-16			T-5-C12E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #1.023 RCHO + #.975 PROD2 + #3.045 XC
	3.70e-13	3.70e-13			T-5-C12E + NO3 = #.547 RO2-R. + #.453 RO2-N. + #.746 R2O2. + #.547 RNO3 + #6 XC + #.453 XN
	2.05e-11	2.05e-11			T-5-C12E + O3P = PROD2 + #6 XC
Trans-5-Dodecene [AP]	6.34e-11	6.34e-11			T-5-C12E + HO. = #.741 RO2-R. + #.259 RO2-N. + #.015 R2O2. + #.011 PROD2 + #6 XC + #1.461 PRD1
	1.15e-16	1.15e-16			T-5-C12E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #3.045 XC + #1.023 PRD2 + #.975 PRD3
	3.70e-13	3.70e-13			T-5-C12E + NO3 = #.547 RO2-R. + #.453 RO2-N. + #.746 R2O2. + #.547 RNO3 + #6 XC + #.453 XN
	2.05e-11	2.05e-11			T-5-C12E + O3P = #6 XC + PRD4
	2.69e-11	2.69e-11			PRD1 + HO. = #.112 RO2-R. + #.042 RO2-N. + #.136 R2O2. + #.845 RCO-O2. + #.026 CO + #.006 HCHO + #.01 CCHO + #.103 RCHO + #.01 MGLY + #-0.179 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.171 HO2. + #1.701 RO2-R. + #.127 RO2-N. + CO + #.873 RCHO + #-1.382 XC
	2.69e-11	2.69e-11			PRD2 + HO. = #.112 RO2-R. + #.042 RO2-N. + #.136 R2O2. + #.845 RCO-O2. + #.026 CO + #.006 HCHO + #.01 CCHO + #.103 RCHO + #.01 MGLY + #-0.179 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.171 HO2. + #1.701 RO2-R. + #.127 RO2-N. + CO + #.873 RCHO + #-1.382 XC
	8.22e-12	8.22e-12			PRD3 + HO. = #.838 RO2-R. + #.162 RO2-N. + #.702 R2O2. + #.013 CO2 + #.159 CCHO + #.241 RCHO + #.376 PROD2 + #.034 MGLY + #.088 BACL + #.141 RCO-OH + #.834 XC
	1.35e-11	1.35e-11			PRD4 + HO. = #.378 RO2-R. + #.564 RO2-N. + #1.474 R2O2. + #.058 RCO-O2. + #.005 HCHO + #.031 CCHO + #.285 RCHO + #.001 MEK + #.325 PROD2 + #.008 HCOOH + #-0.442 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Trans-5-Tridecene [LP]	6.34e-11	6.34e-11			T-5-C13E + HO. = #.735 RO2-R. + #.265 RO2-N. + #.015 R2O2. + #1.449 RCHO + #.011 PROD2 + #7 XC
	1.15e-16	1.15e-16			T-5-C13E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #1.023 RCHO + #.975 PROD2 + #4.045 XC
	3.70e-13	3.70e-13			T-5-C13E + NO3 = #.538 RO2-R. + #.462 RO2-N. + #.753 R2O2. + #.538 RNO3 + #7 XC + #.462 XN
	2.05e-11	2.05e-11			T-5-C13E + O3P = PROD2 + #7 XC
Trans-5-Tridecene [AP]	6.34e-11	6.34e-11			T-5-C13E + HO. = #.735 RO2-R. + #.265 RO2-N. + #.015 R2O2. + #.011 PROD2 + #7 XC + #1.449 PRD1
	1.15e-16	1.15e-16			T-5-C13E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #4.045 XC + #1.023 PRD2 + #.975 PRD3
	3.70e-13	3.70e-13			T-5-C13E + NO3 = #.538 RO2-R. + #.462 RO2-N. + #.753 R2O2. + #.538 RNO3 + #7 XC + #.462 XN
	2.05e-11	2.05e-11			T-5-C13E + O3P = #7 XC + PRD4
	2.77e-11	2.77e-11			PRD1 + HO. = #.126 RO2-R. + #.057 RO2-N. + #.149 R2O2. + #.817 RCO-O2. + #.025 CO + #.006 HCHO + #.01 CCHO + #.118 RCHO + #.009 MGLY + #-0.223 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.19 HO2. + #1.649 RO2-R. + #.161 RO2-N. + CO + #.839 RCHO + #-1.482 XC
	2.77e-11	2.77e-11			PRD2 + HO. = #.126 RO2-R. + #.057 RO2-N. + #.149 R2O2. + #.817 RCO-O2. + #.025 CO + #.006 HCHO + #.01 CCHO + #.118 RCHO + #.009 MGLY + #-0.223 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.19 HO2. + #1.649 RO2-R. + #.161 RO2-N. + CO + #.839 RCHO + #-1.482 XC
	8.94e-12	8.94e-12			PRD3 + HO. = #.801 RO2-R. + #.199 RO2-N. + #.691 R2O2. + #.008 CO2 + #.159 CCHO + #.216 RCHO + #.362 PROD2 + #.034 MGLY + #.082 BACL + #.141 RCO-OH + #.807 XC
	1.49e-11	1.49e-11			PRD4 + HO. = #.368 RO2-R. + #.581 RO2-N. + #1.444 R2O2. + #.05 RCO-O2. + #.005 HCHO + #.028 CCHO + #.252 RCHO + #.001 MEK + #.319 PROD2 + #.007 HCOOH + #-0.383 XC
Trans-5-Tetra-decene [LP]	6.34e-11	6.34e-11			T-5-C14E + HO. = #.732 RO2-R. + #.268 RO2-N. + #.015 R2O2. + #1.442 RCHO + #.011 PROD2 + #8 XC
	1.15e-16	1.15e-16			T-5-C14E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #1.023 RCHO + #.975 PROD2 + #5.045 XC
	3.70e-13	3.70e-13			T-5-C14E + NO3 = #.533 RO2-R. + #.467 RO2-N. + #.753 R2O2. + #.533 RNO3 + #8 XC + #.467 XN
	2.05e-11	2.05e-11			T-5-C14E + O3P = PROD2 + #8 XC
Trans-5-Tetradecene [AP]	6.34e-11	6.34e-11			T-5-C14E + HO. = #.732 RO2-R. + #.268 RO2-N. + #.015 R2O2. + #.011 PROD2 + #8 XC + #1.442 PRD1
	1.15e-16	1.15e-16			T-5-C14E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #5.045 XC + #1.023 PRD2 + #.975 PRD3
	3.70e-13	3.70e-13			T-5-C14E + NO3 = #.533 RO2-R. + #.467 RO2-N. + #.753 R2O2. + #.533 RNO3 + #8 XC + #.467 XN
	2.05e-11	2.05e-11			T-5-C14E + O3P = #8 XC + PRD4
	2.84e-11	2.84e-11			PRD1 + HO. = #.134 RO2-R. + #.07 RO2-N. + #.162 R2O2. + #.796 RCO-O2. + #.025 CO + #.006 HCHO + #.01 CCHO + #.126 RCHO + #.007 MGLY + #-0.262 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.164 HO2. + #1.636 RO2-R. + #.201 RO2-N. + CO + #.761 RCHO + #.038 PROD2 + #-1.716 XC
	2.84e-11	2.84e-11			PRD2 + HO. = #.134 RO2-R. + #.07 RO2-N. + #.162 R2O2. + #.796 RCO-O2. + #.025 CO + #.006 HCHO + #.01 CCHO + #.126 RCHO + #.007 MGLY + #-0.262 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.164 HO2. + #1.636 RO2-R. + #.201 RO2-N. + CO + #.761 RCHO + #.038 PROD2 + #-1.716 XC
	9.67e-12	9.67e-12			PRD3 + HO. = #.773 RO2-R. + #.227 RO2-N. + #.681 R2O2. + #.008 CO2 + #.159 CCHO + #.213 RCHO + #.344 PROD2 + #.034 MGLY + #.074 BACL + #.141 RCO-OH + #.783 XC
	1.63e-11	1.63e-11			PRD4 + HO. = #.379 RO2-R. + #.579 RO2-N. + #1.357 R2O2. + #.043 RCO-O2. + #.004 HCHO + #.025 CCHO + #.188 RCHO + #.35 PROD2 + #.005 HCOOH + #-0.327 XC
Trans-5-Tetra-decene [LP]	6.34e-11	6.34e-11			T-5-C15E + HO. = #.729 RO2-R. + #.271 RO2-N. + #.015 R2O2. + #1.437 RCHO + #.01 PROD2 + #9 XC
	1.15e-16	1.15e-16			T-5-C15E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #1.023 RCHO + #.975 PROD2 + #6.045 XC
	3.70e-13	3.70e-13			T-5-C15E + NO3 = #.53 RO2-R. + #.47 RO2-N. + #.752 R2O2. + #.53 RNO3 + #9 XC + #.47 XN
	2.05e-11	2.05e-11			T-5-C15E + O3P = PROD2 + #9 XC
Trans-5-Tetra-decene [AP]	6.34e-11	6.34e-11			T-5-C15E + HO. = #.729 RO2-R. + #.271 RO2-N. + #.015 R2O2. + #.01 PROD2 + #9 XC + #1.437 PRD1
	1.15e-16	1.15e-16			T-5-C15E + O3 = #.025 HO. + #.023 RO2-R. + #.002 RO2-N. + #.019 R2O2. + #.025 CO + #6.045 XC + #1.023 PRD2 + #.975 PRD3
	3.70e-13	3.70e-13			T-5-C15E + NO3 = #.53 RO2-R. + #.47 RO2-N. + #.752 R2O2. + #.53 RNO3 + #9 XC + #.47 XN
	2.05e-11	2.05e-11			T-5-C15E + O3P = #9 XC + PRD4
	2.91e-11	2.91e-11			PRD1 + HO. = #.139 RO2-R. + #.082 RO2-N. + #.174 R2O2. + #.779 RCO-O2. + #.024 CO + #.006 HCHO + #.01 CCHO + #.133 RCHO + #.006 MGLY + #-0.297 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.171 HO2. + #1.598 RO2-R. + #.231 RO2-N. + CO + #.726 RCHO + #.043 PROD2 + #-1.823 XC
	2.91e-11	2.91e-11			PRD2 + HO. = #.139 RO2-R. + #.082 RO2-N. + #.174 R2O2. + #.779 RCO-O2. + #.024 CO + #.006 HCHO + #.01 CCHO + #.133 RCHO + #.006 MGLY + #-0.297 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.171 HO2. + #1.598 RO2-R. + #.231 RO2-N. + CO + #.726 RCHO + #.043 PROD2 + #-1.823 XC
	1.04e-11	1.04e-11			PRD3 + HO. = #.752 RO2-R. + #.248 RO2-N. + #.677 R2O2. + #.008 CO2 + #.159 CCHO + #.214 RCHO + #.326 PROD2 + #.034 MGLY + #.07 BACL + #.141 RCO-OH + #.779 XC
	1.77e-11	1.77e-11			PRD4 + HO. = #.394 RO2-R. + #.567 RO2-N. + #1.272 R2O2. + #.039 RCO-O2. + #.004 HCHO + #.023 CCHO + #.169 RCHO + #.368 PROD2 + #.005 HCOOH + #-0.293 XC
Cyclopentene [LP]	6.70e-11	1.25e-11	-0.99		CYC-PNTE + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 RCHO + #1.805 XC
	5.56e-16	1.80e-15	0.70		CYC-PNTE + O3 = #.05 HO. + #.002 RO2-N. + #.048 R2O2. + #.048 RCO-O2. + #.05 CO + #.95 RCHO + #1.944 XC
	5.30e-13	5.30e-13			CYC-PNTE + NO3 = #.812 NO2 + #.064 RO2-R. + #.125 RO2-N. + #.949 R2O2. + #.787 RCHO + #.077 MGLY + #.012 RNO3 + #1.59 XC + #.177 XN
	2.10e-11	2.10e-11			CYC-PNTE + O3P = #.24 MEK + #.76 PROD2 + #-0.52 XC
Cyclopentene [AP]	6.70e-11	1.25e-11	-0.99		CYC-PNTE + HO. = #.935 RO2-R. + #.065 RO2-N. + #1.805 XC + #.935 PRD1
	5.56e-16	1.80e-15	0.70		CYC-PNTE + O3 = #.05 HO. + #.002 RO2-N. + #.048 R2O2. + #.048 RCO-O2. + #.05 CO + #1.944 XC + #.95 PRD2
	5.30e-13	5.30e-13			CYC-PNTE + NO3 = #.812 NO2 + #.064 RO2-R. + #.125 RO2-N. + #.949 R2O2. + #.012 RNO3 + #1.59 XC + #.787 PRD3 + #.077 PRD4 + #.177 XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.10e-11	2.10e-11			CYC-PNTE + O3P = #.24 MEK + #-0.52 XC + #.76 PRD5
	4.16e-11	4.16e-11			PRD1 + HO. = #.04 RO2-R. + #.009 RO2-N. + #.051 R2O2. + #.951 RCO-O2. + #.033 CO + #.023 HCHO + #.04 RCHO + #.001 GLY + #-0.085 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 RCO-O2. + CO + #-1.118 XC
	2.55e-11	2.55e-11			PRD2 + HO. = #.196 RO2-R. + #.016 RO2-N. + #.154 R2O2. + #.788 RCO-O2. + #.111 CO + #.079 HCHO + #.196 RCHO + #.004 GLY + #.04 MGLY + #-0.364 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.987 HO2. + #.973 RO2-R. + #.039 RO2-N. + CO + #.013 HCHO + #.961 RCHO + #-1.131 XC
	4.16e-11	4.16e-11			PRD3 + HO. = #.002 NO2 + #.038 RO2-R. + #.009 RO2-N. + #.05 R2O2. + #.951 RCO-O2. + #.032 CO + #.022 HCHO + #.04 RCHO + #.003 GLY + #-0.085 XC + #.064 XN
	7.60e-15	7.60e-15			PRD3 + NO3 = RCO-O2. + #1.066 XN
		PF=C2CHO			PRD3 + HV = #.033 NO2 + #.071 HO2. + #.929 RO2-R. + #.038 RO2-N. + #.929 RCO-O2. + CO + #.033 RCHO + #-1.114 XC + #.033 XN
	2.13e-11	2.13e-11			PRD4 + HO. = #.153 HO2. + #.236 RO2-R. + #.016 RO2-N. + #.594 RCO-O2. + #.198 HCHO + #.037 RCHO + #.39 MGLY + #-0.358 XC
	2.53e-15	2.53e-15			PRD4 + NO3 = RCO-O2. + XN
		PF=MGLY_ADJ			PRD4 + HV = HO2. + RCO-O2. + CO + #-1 XC
	5.06e-12	5.06e-12			PRD5 + HO. = #.776 RO2-R. + #.224 RO2-N. + #1.661 R2O2. + #.054 CO + #.756 RCHO + #.02 MEK + #2.255 XC
1-Methyl cyclohexene [LP]	8.71e-11	8.71e-11			1M-CC5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 RCHO + #2.707 XC
	6.70e-16	2.70e-15	0.83		1M-CC5E + O3 = #.7 HO. + #.068 RO2-N. + #.632 R2O2. + #.564 CCO-O2. + #.068 RCO-O2. + #.068 HCHO + #.564 RCHO + #.3 PROD2 + #.699 XC
	9.37e-12	9.37e-12			1M-CC5E + NO3 = #.837 NO2 + #.052 RO2-R. + #.111 RO2-N. + #.979 R2O2. + #.812 RCHO + #.077 BACL + #2.589 XC + #.163 XN
	3.71e-11	3.71e-11			1M-CC5E + O3P = PROD2
1-Methyl cyclohexene [AP]	8.71e-11	8.71e-11			1M-CC5E + HO. = #.902 RO2-R. + #.098 RO2-N. + #2.707 XC + #.902 PRD1
	6.70e-16	2.70e-15	0.83		1M-CC5E + O3 = #.7 HO. + #.068 RO2-N. + #.632 R2O2. + #.564 CCO-O2. + #.068 RCO-O2. + #.068 HCHO + #.699 XC + #.3 PRD2 + #.564 PRD3
	9.37e-12	9.37e-12			1M-CC5E + NO3 = #.837 NO2 + #.052 RO2-R. + #.111 RO2-N. + #.979 R2O2. + #2.589 XC + #.812 PRD4 + #.077 PRD5 + #.163 XN
	3.71e-11	3.71e-11			1M-CC5E + O3P = PRD6
	2.55e-11	2.55e-11			PRD1 + HO. = #.071 RO2-R. + #.024 RO2-N. + #.294 R2O2. + #.149 CCO-O2. + #.756 RCO-O2. + #.056 CO + #.144 HCHO + #.22 RCHO + #.001 GLY + #-0.572 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.987 HO2. + #.947 RO2-R. + #.065 RO2-N. + CO + #.013 HCHO + #.934 RCHO + #-1.209 XC
	1.60e-11	1.60e-11			PRD2 + HO. = #.196 RO2-R. + #.098 RO2-N. + #1.434 R2O2. + #.706 CCO-O2. + #.005 CO2 + #.657 HCHO + #.783 RCHO + #.071 MGLY + #.044 BACL + #.076 RCO-OH + #.375 XC
		PF=KETONE QY = 2.0e-2			PRD2 + HV = #.961 RO2-R. + #.039 RO2-N. + #.013 R2O2. + CCO-O2. + #.013 HCHO + #.961 RCHO + #.869 XC
	4.02e-11	4.02e-11			PRD3 + HO. = #.04 RO2-R. + #.003 RO2-N. + #.957 RCO-O2. + #.04 CO + #.04 RCHO + #-0.05 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	7.60e-15	7.60e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = HO2. + RO2-R. + CO + RCHO + #-1 XC
	2.55e-11	2.55e-11			PRD4 + HO. = #.009 NO2 + #.07 RO2-R. + #.024 RO2-N. + #.285 R2O2. + #.139 CCO-O2. + #.758 RCO-O2. + #.056 CO + #.136 HCHO + #.219 RCHO + #.001 GLY + #.009 MGLY + #-0.571 XC + #.055 XN
	3.80e-15	3.80e-15			PRD4 + NO3 = RCO-O2. + #-0 XC + #1.064 XN
		PF=C2CHO			PRD4 + HV = #.987 HO2. + #.947 RO2-R. + #.065 RO2-N. + CO + #.013 HCHO + #.934 RCHO + #-1.209 XC + #.064 XN
	9.63e-12	9.63e-12			PRD5 + HO. = #.347 HO2. + #.513 RO2-R. + #.055 RO2-N. + #.085 RCO-O2. + #.423 HCHO + #.081 RCHO + #.003 MGLY + #.857 BACL + #-0.688 XC
		PF=BACL_ADJ			PRD5 + HV = CCO-O2. + RCO-O2. + #-1 XC
	6.59e-12	6.59e-12			PRD6 + HO. = #.307 RO2-R. + #.254 RO2-N. + #1.757 R2O2. + #.144 CCO-O2. + #.296 RCO-O2. + #.014 CO + #.117 HCHO + #.186 CCHO + #.449 RCHO + #.002 PROD2 + #.001 GLY + #1.441 XC
		PF=KETONE QY = 2.0e-2			PRD6 + HV = #5 XC
Cyclohexene [LP]	6.75e-11	1.26e-11	-0.99		CYC-HEXE + HO. = #.902 RO2-R. + #.098 RO2-N. + #.902 RCHO + #2.707 XC
	8.14e-17	2.88e-15	2.11		CYC-HEXE + O3 = RCHO + #3 XC
	5.85e-13	1.05e-12	0.35		CYC-HEXE + NO3 = #.296 NO2 + #.539 RO2-R. + #.165 RO2-N. + #.401 R2O2. + #.341 RCHO + #.494 RNO3 + #1.024 XC + #.21 XN
	2.00e-11	2.00e-11			CYC-HEXE + O3P = PROD2
Cyclohexene [AP]	6.75e-11	1.26e-11	-0.99		CYC-HEXE + HO. = #.902 RO2-R. + #.098 RO2-N. + #2.707 XC + #.902 PRD1
	8.14e-17	2.88e-15	2.11		CYC-HEXE + O3 = #3 XC + PRD2
	5.85e-13	1.05e-12	0.35		CYC-HEXE + NO3 = #.296 NO2 + #.539 RO2-R. + #.165 RO2-N. + #.401 R2O2. + #.494 RNO3 + #1.024 XC + #.341 PRD3 + #.21 XN
	2.00e-11	2.00e-11			CYC-HEXE + O3P = PRD4
	4.30e-11	4.30e-11			PRD1 + HO. = #.033 RO2-R. + #.018 RO2-N. + #.075 R2O2. + #.948 RCO-O2. + #.016 CO + #.018 RCHO + #.016 MGLY + #-0.074 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.078 HO2. + #1.798 RO2-R. + #.125 RO2-N. + #1.063 CO + #.875 RCHO + #-1.437 XC
	2.69e-11	2.69e-11			PRD2 + HO. = #.104 RO2-R. + #.032 RO2-N. + #.233 R2O2. + #.864 RCO-O2. + #.018 CO + #.004 HCHO + #.102 RCHO + #.015 MGLY + #.025 BACL + #-0.254 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.078 HO2. + #1.797 RO2-R. + #.125 RO2-N. + CO + #.875 RCHO + #-1.374 XC
	4.41e-11	4.41e-11			PRD3 + HO. = #.026 HO2. + #.034 RO2-R. + #.016 RO2-N. + #.065 R2O2. + #.923 RCO-O2. + #.016 CO + #.051 RCHO + #.014 MGLY + #-0.078 XC + #.132 XN
	7.60e-15	7.60e-15			PRD3 + NO3 = RCO-O2. + #1.132 XN
		PF=C2CHO			PRD3 + HV = #.103 NO2 + #.163 HO2. + #1.622 RO2-R. + #.113 RO2-N. + #1.055 CO + #.851 RCHO + #.037 MGLY + #-1.392 XC + #.029 XN
	7.05e-12	7.05e-12			PRD4 + HO. = #.7 RO2-R. + #.195 RO2-N. + #.533 R2O2. + #.105 RCO-O2. + #.014 HCHO + #.2 RCHO + #.501 PROD2 + #.894 XC
		PF=KETONE QY = 1.2e-2			PRD4 + HV = #6 XC
1-Methyl Cyclohexene [LP]	8.71e-11	8.71e-11			1M-CC6E + HO. = #.865 RO2-R. + #.135 RO2-N. + #.865 RCHO + #3.595 XC
	1.65e-16	2.87e-15	1.69		1M-CC6E + O3 = #.7 HO. + #.095 RO2-N. + #.605 R2O2. + #.54 CCO-O2. + #.065 RCO-O2. + #.065 HCHO + #.54 RCHO + #.3 PROD2 + #1.67 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	9.37e-12	9.37e-12			1M-CC6E + NO3 = #.729 NO2 + #.102 RO2-R. + #.169 RO2-N. + #.983 R2O2. + #.831 RCHO + #3.492 XC + #.271 XN
	9.00e-11	9.00e-11			1M-CC6E + O3P = PROD2 + XC
1-Methyl Cyclohexene [AP]	8.71e-11	8.71e-11			1M-CC6E + HO. = #.865 RO2-R. + #.135 RO2-N. + #3.595 XC + #.865 PRD1
	1.65e-16	2.87e-15	1.69		1M-CC6E + O3 = #.7 HO. + #.095 RO2-N. + #.605 R2O2. + #.54 CCO-O2. + #.065 RCO-O2. + #.065 HCHO + #1.67 XC + #.3 PRD2 + #.54 PRD3
	9.37e-12	9.37e-12			1M-CC6E + NO3 = #.729 NO2 + #.102 RO2-R. + #.169 RO2-N. + #.983 R2O2. + #3.492 XC + #.831 PRD4 + #.271 XN
	9.00e-11	9.00e-11			1M-CC6E + O3P = XC + PRD5
	2.70e-11	2.70e-11			PRD1 + HO. = #.059 RO2-R. + #.042 RO2-N. + #.239 R2O2. + #.042 CCO-O2. + #.857 RCO-O2. + #.016 CO + #.005 HCHO + #.136 RCHO + #-0.335 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #1.012 RO2-R. + #.184 RO2-N. + #.693 R2O2. + #.803 CCO-O2. + CO + #.816 RCHO + #-3.16 XC
	1.09e-11	1.09e-11			PRD2 + HO. = #.606 RO2-R. + #.155 RO2-N. + #.902 R2O2. + #.239 CCO-O2. + #.113 HCHO + #1.175 RCHO + #.136 PROD2 + #.015 MGLY + #.094 XC
		PF=KETONE QY = 1.0e-2			PRD2 + HV = #.875 RO2-R. + #.125 RO2-N. + #.922 R2O2. + CCO-O2. + #.875 RCHO + #.626 XC
	4.16e-11	4.16e-11			PRD3 + HO. = #.04 RO2-R. + #.009 RO2-N. + #.051 R2O2. + #.951 RCO-O2. + #.033 CO + #.023 HCHO + #.04 RCHO + #.001 GLY + #-0.085 XC
	7.60e-15	7.60e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 RCO-O2. + CO + #-1.118 XC
	3.03e-11	3.03e-11			PRD4 + HO. = #.073 HO2. + #.056 RO2-R. + #.037 RO2-N. + #.209 R2O2. + #.037 CCO-O2. + #.796 RCO-O2. + #.016 CO + #.004 HCHO + #.2 RCHO + #-0.306 XC + #.123 XN
	3.80e-15	3.80e-15			PRD4 + NO3 = RCO-O2. + #-0 XC + #1.123 XN
		PF=C2CHO			PRD4 + HV = #.066 NO2 + #.057 HO2. + #.999 RO2-R. + #.174 RO2-N. + #.608 R2O2. + #.705 CCO-O2. + CO + #.76 RCHO + #.066 BACL + #-2.997 XC + #.057 XN
	1.14e-11	1.14e-11			PRD5 + HO. = #.507 RO2-R. + #.293 RO2-N. + #1.147 R2O2. + #.2 RCO-O2. + #.04 HCHO + #.106 CCHO + #.324 RCHO + #.187 PROD2 + #1.296 XC
		PF=KETONE QY = 8.0e-3			PRD5 + HV = #5 XC
4-Methyl Cyclohexene [LP]	6.34e-11	6.34e-11			4M-CC6E + HO. = #.865 RO2-R. + #.135 RO2-N. + #.865 RCHO + #3.595 XC
	8.21e-17	2.88e-15	2.11		4M-CC6E + O3 = RCHO + #4 XC
	3.70e-13	3.70e-13			4M-CC6E + NO3 = #.264 NO2 + #.519 RO2-R. + #.218 RO2-N. + #.468 R2O2. + #.003 HCHO + #.003 CCHO + #.343 RCHO + #.003 PROD2 + #.44 RNO3 + #2 XC + #.296 XN
	2.05e-11	2.05e-11			4M-CC6E + O3P = PROD2 + XC
4-Methyl Cyclohexene [AP]	6.34e-11	6.34e-11			4M-CC6E + HO. = #.865 RO2-R. + #.135 RO2-N. + #3.595 XC + #.865 PRD1
	8.21e-17	2.88e-15	2.11		4M-CC6E + O3 = #4 XC + PRD2
	3.70e-13	3.70e-13			4M-CC6E + NO3 = #.264 NO2 + #.519 RO2-R. + #.218 RO2-N. + #.468 R2O2. + #.003 HCHO + #.003 CCHO + #.003 PROD2 + #.44 RNO3 + #2 XC + #.343 PRD3 + #.296 XN
	2.05e-11	2.05e-11			4M-CC6E + O3P = XC + PRD4

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	4.47e-11	4.47e-11			PRD1 + HO. = #.058 RO2-R. + #.027 RO2-N. + #.108 R2O2. + #.915 RCO-O2. + #.02 CO + #.007 HCHO + #.006 CCHO + #.067 RCHO + #.016 MGLY + #-0.192 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.1 HO2. + #1.707 RO2-R. + #.185 RO2-N. + #.009 RCO-O2. + #1.049 CO + #.006 HCHO + #.806 RCHO + #-1.608 XC
	3.02e-11	3.02e-11			PRD2 + HO. = #.179 RO2-R. + #.059 RO2-N. + #.317 R2O2. + #.762 RCO-O2. + #.03 CO + #.019 HCHO + #.019 CCHO + #.222 RCHO + #.005 PROD2 + #.001 GLY + #.016 MGLY + #.02 BACL + #.036 RCO-OH + #-0.66 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.107 HO2. + #1.709 RO2-R. + #.184 RO2-N. + CO + #.006 HCHO + #.002 CCHO + #.813 RCHO + #.003 PROD2 + #-1.573 XC
	4.61e-11	4.61e-11			PRD3 + HO. = #.035 HO2. + #.058 RO2-R. + #.023 RO2-N. + #.088 R2O2. + #.884 RCO-O2. + #.022 CO + #.005 HCHO + #.005 CCHO + #.104 RCHO + #.013 MGLY + #-0.179 XC + #.183 XN
	7.60e-15	7.60e-15			PRD3 + NO3 = RCO-O2. + #1.183 XN
		PF=C2CHO			PRD3 + HV = #.129 NO2 + #.199 HO2. + #1.5 RO2-R. + #.161 RO2-N. + #.011 RCO-O2. + #1.04 CO + #.025 HCHO + #.024 CCHO + #.791 RCHO + #.037 MGLY + #-1.596 XC + #.054 XN
	1.13e-11	1.13e-11			PRD4 + HO. = #.627 RO2-R. + #.32 RO2-N. + #1.157 R2O2. + #.054 RCO-O2. + #.045 HCHO + #.032 CCHO + #.472 RCHO + #.164 PROD2 + #.002 GLY + #1.406 XC
		PF=KETONE QY = 4.8e-3			PRD4 + HV = #5.5 XC
1,2-Dimethyl Cyclohexene [LP]	1.05e-10	1.05e-10			12M-CC6E + HO. = #.827 RO2-R. + #.173 RO2-N. + #.827 PROD2 + #2 XC
	2.07e-16	3.03e-15	1.59		12M-CC6E + O3 = HO. + #.173 RO2-N. + #.827 R2O2. + #.738 CCO-O2. + #.089 RCO-O2. + #.089 HCHO + #.738 RCHO + #2.915 XC
	5.72e-11	5.72e-11			12M-CC6E + NO3 = #.827 NO2 + #.173 RO2-N. + #.827 R2O2. + #.827 PROD2 + #2 XC + #.173 XN
	5.29e-11	5.29e-11			12M-CC6E + O3P = PROD2 + #2 XC
1,2-Dimethyl Cyclohexene [AP]	1.05e-10	1.05e-10			12M-CC6E + HO. = #.827 RO2-R. + #.173 RO2-N. + #2 XC + #.827 PRD1
	2.07e-16	3.03e-15	1.59		12M-CC6E + O3 = HO. + #.173 RO2-N. + #.827 R2O2. + #.738 CCO-O2. + #.089 RCO-O2. + #.089 HCHO + #2.915 XC + #.738 PRD2
	5.72e-11	5.72e-11			12M-CC6E + NO3 = #.827 NO2 + #.173 RO2-N. + #.827 R2O2. + #2 XC + #.827 PRD1 + #.173 XN
	5.29e-11	5.29e-11			12M-CC6E + O3P = #2 XC + PRD3
	1.09e-11	1.09e-11			PRD1 + HO. = #.463 RO2-R. + #.188 RO2-N. + #.925 R2O2. + #.333 CCO-O2. + #.016 RCO-O2. + #.223 HCHO + #1.057 RCHO + #.108 PROD2 + #.113 XC
		PF=KETONE QY = 1.0e-2			PRD1 + HV = #.012 RO2-R. + #.184 RO2-N. + #1.693 R2O2. + #1.803 CCO-O2. + #.816 RCHO + #-1.16 XC
	2.55e-11	2.55e-11			PRD2 + HO. = #.071 RO2-R. + #.024 RO2-N. + #.294 R2O2. + #.149 CCO-O2. + #.756 RCO-O2. + #.056 CO + #.144 HCHO + #.22 RCHO + #.001 GLY + #-0.572 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.987 HO2. + #.947 RO2-R. + #.065 RO2-N. + CO + #.013 HCHO + #.934 RCHO + #-1.209 XC
	1.19e-11	1.19e-11			PRD3 + HO. = #.57 RO2-R. + #.43 RO2-N. + #1.36 R2O2. + #.001 CO + #.037 HCHO + #.078 CCHO + #.197 RCHO + #.381 PROD2 + #.352 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
1,3-Butadiene [LP]	6.65e-11	1.48e-11	-0.89		13-BUTDE + HO. = #.961 RO2-R. + #.039 RO2-N. + #.48 HCHO + #.48 METHACRO + #.48 ISO-PROD + #-1.039 XC
	6.31e-18	1.34e-14	4.54		13-BUTDE + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.19 CO2 + #.5 HCHO + #.125 PROD2 + #.5 METHACRO + #.375 MVK + #.185 HCOOH + #-1.375 XC
	1.00e-13	1.00e-13			13-BUTDE + NO3 = #.92 RO2-R. + #.08 RO2-N. + #.92 MVK + #-0.161 XC + XN
	1.98e-11	1.98e-11			13-BUTDE + O3P = #.25 HO2. + #.23 RO2-R. + #.02 RO2-N. + #.23 CO + #.75 PROD2 + #.23 METHACRO + #-1.77 XC
1,3-Butadiene [AP]	6.65e-11	1.48e-11	-0.89		13-BUTDE + HO. = #.961 RO2-R. + #.039 RO2-N. + #.48 HCHO + #-1.039 XC + #.48 PRD1 + #.48 PRD2
	6.31e-18	1.34e-14	4.54		13-BUTDE + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.19 CO2 + #.5 HCHO + #.185 HCOOH + #-1.375 XC + #.5 PRD1 + #.125 PRD3 + #.375 PRD4
	1.00e-13	1.00e-13			13-BUTDE + NO3 = #.92 RO2-R. + #.08 RO2-N. + #-0.161 XC + #.92 PRD5 + XN
	1.98e-11	1.98e-11			13-BUTDE + O3P = #.25 HO2. + #.23 RO2-R. + #.02 RO2-N. + #.23 CO + #-1.77 XC + #.23 PRD1 + #.75 PRD6
	1.99e-11	1.99e-11			PRD1 + HO. = #.25 RO2-R. + #.75 MA-RCO3. + #.167 CO + #.083 HCHO + #.167 CCHO + #.083 GLY + #.25 XC
	3.07e-19	3.07e-19			PRD1 + O3 = #.31 HO. + #.81 HO2. + CO + #.315 CO2 + #.5 HCHO + #.5 GLY + #.185 HCOOH + XC
	2.94e-15	2.94e-15			PRD1 + NO3 = #.031 RO2-R. + #.002 RO2-N. + #.967 MA-RCO3. + #.031 CO + #.031 RCHO + #-0.003 XC + XN
	2.37e-12	2.37e-12			PRD1 + O3P = RCHO + XC
	PF=ACROLEIN QY = 2.0e-3				PRD1 + HV = #.172 HO. + #1.01 HO2. + #.172 C-O2. + #.33 MA-RCO3. + #1.182 CO + #.046 CO2 + #.34 HCHO + #.112 CCO-OH + #.716 XC
	2.16e-11	2.16e-11			PRD2 + HO. = #.961 RO2-R. + #.039 RO2-N. + #.467 CO + #.043 HCHO + #.451 CCHO + #.51 RCHO + #.451 GLY + #.921 XC
	1.15e-16	1.15e-16			PRD2 + O3 = #.306 HO. + #.806 HO2. + #.806 CO + #.25 CO2 + #.057 HCHO + #.5 CCHO + #.5 GLY + #.444 RCO-OH + #.557 XC
	5.43e-15	5.43e-15			PRD2 + NO3 = #.458 RO2-R. + #.019 RO2-N. + #.523 MA-RCO3. + #.229 CO + #.229 HCHO + #.458 RCHO + #.962 XC + XN
	2.75e-12	2.75e-12			PRD2 + O3P = #.88 RCHO + #.12 MGLY + #2 XC
	PF=ACROLEIN QY = 4.1e-3				PRD2 + HV = #2 HO2. + #2 CO + CCHO + XC
	8.43e-12	8.43e-12			PRD3 + HO. = RO2-R. + #1.611 HCHO + #.195 CCHO + #4 XC
	1.68e-18	1.68e-18			PRD3 + O3 = #.12 HO. + #.12 HO2. + #.5 CO + #.13 CO2 + HCHO + #.37 HCOOH + #4 XC
	2.18e-16	2.18e-16			PRD3 + NO3 = RO2-R. + RCHO + #3 XC + XN
	7.42e-13	7.42e-13			PRD3 + O3P = #.5 HO2. + #.2 RO2-R. + #.3 C-O2. + #.491 CO + #.191 HCHO + #.25 CCHO + #.009 GLY + #4.25 XC
	2.84e-11	2.84e-11			PRD4 + HO. = RO2-R. + #.015 CO2 + #.548 HCHO + #.015 CCHO + #.208 RCHO + #.548 MGLY + #.229 BACL + #.223 XC
	1.01e-17	1.01e-17			PRD4 + O3 = #.11 HO. + #.11 HO2. + #.3 CO + #.115 CO2 + #.5 HCHO + #.5 MGLY + #.185 HCOOH + #.95 XC
	2.76e-18	2.76e-18			PRD4 + NO3 = RO2-R. + #.062 CO2 + #.062 RCHO + #.938 BACL + XN
	4.60e-12	4.60e-12			PRD4 + O3P = #.45 RCHO + #.55 RCO-OH + XC
	2.84e-11	2.84e-11			PRD5 + HO. = #.337 RO2-R. + #.039 RO2-N. + #.623 R2O2. + #.623 RCO-O2. + #.199 HCHO + #.623 CCHO + #.138 RCHO + #.199 MGLY + #-0.564 XC + XN
	1.01e-17	1.01e-17			PRD5 + O3 = #.5 NO2 + #.56 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + MGLY + #.185 HCOOH + #.5 XN
	2.76e-18	2.76e-18			PRD5 + NO3 = #.039 RO2-N. + #.961 R2O2. + #.961 RCO-O2. + #.961 RCHO + #-2 XC + #2 XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	4.60e-12	4.60e-12			PRD5 + O3P = #.45 RCHO + #.55 RNO3 + #-0.65 XC + #.45 XN
	PF=ACROLEIN QY = 2.1e-3				PRD5 + HV = #.5 NO2 + #.5 HO2. + #.5 RCO-O2. + #.5 MA-RCO3. + #.5 CO + HCHO + #-1 XC + #.5 XN
	3.16e-11	3.16e-11			PRD6 + HO. = #.888 RO2-R. + #.057 RO2-N. + #1.597 R2O2. + #.055 RCO-O2. + #.227 CO + #.043 CO2 + #.225 HCHO + #.696 CCHO + #.189 RCHO + #.003 PROD2 + #.283 HCOOH + #2.311 XC
	1.01e-17	1.01e-17			PRD6 + O3 = #.101 HO. + #.019 HO2. + #.082 RO2-R. + #.308 CO + #.068 CO2 + #.503 HCHO + #.5 RCHO + #.202 HCOOH + #.46 RCO-OH + #2.02 XC
	1.38e-14	1.38e-14			PRD6 + NO3 = #.961 RO2-R. + #.039 RO2-N. + #1.921 R2O2. + #.394 CO + #.068 CO2 + #.068 HCHO + #.961 RCHO + #.394 HCOOH + #1.458 XC + XN
	5.60e-12	5.60e-12			PRD6 + O3P = #.45 RCHO + #.55 MEK + #2.45 XC
Isoprene	1.01e-10	2.55e-11	-0.82		ISOPRENE + HO. = #.907 RO2-R. + #.093 RO2-N. + #.079 R2O2. + #.624 HCHO + #.23 METHACRO + #.32 MVK + #.357 ISO-PROD + #-0.167 XC
	1.28e-17	7.86e-15	3.80		ISOPRENE + O3 = #.266 HO. + #.066 RO2-R. + #.008 RO2-N. + #.126 R2O2. + #.192 MA-RCO3. + #.275 CO + #.122 CO2 + #.592 HCHO + #.1 PROD2 + #.39 METHACRO + #.16 MVK + #.15 ISO-PROD + #.204 HCOOH + #-0.558 XC
	6.79e-13	3.03e-12	0.89		ISOPRENE + NO3 = #.187 NO2 + #.748 RO2-R. + #.065 RO2-N. + #.187 R2O2. + #.935 ISO-PROD + #-0.065 XC + #.813 XN
	3.60e-11	3.60e-11			ISOPRENE + O3P = #.01 RO2-N. + #.24 R2O2. + #.25 C-O2. + #.24 MA-RCO3. + #.24 HCHO + #.75 PROD2 + #-1.01 XC
3-Carene [PM]	8.79e-11	1.64e-11	-0.99	0.0	3-CARENE + HO. = #.75 RO2-R. + #.25 RO2-N. + #.5 R2O2. + #.75 RCHO + #6.25 XC
	3.70e-17	1.01e-15	1.96	0.0	3-CARENE + O3 = #.7 HO. + #.161 RO2-N. + #.539 R2O2. + #.482 CCO-O2. + #.058 RCO-O2. + #.058 HCHO + #.482 RCHO + #.3 RCO-OH + #5.492 XC
	9.10e-12	9.10e-12	0.00	0.0	3-CARENE + NO3 = #.75 NO2 + #.25 RO2-N. + #.75 R2O2. + #.75 RCHO + #6.25 XC + #.25 XN
	3.20e-11	3.20e-11	0.00	0.0	3-CARENE + O3P = PROD2 + #4 XC
a-Pinene [PM]	5.37e-11	1.21e-11	-0.88	0.0	A-PINENE + HO. = #.75 RO2-R. + #.25 RO2-N. + #.5 R2O2. + #.75 RCHO + #6.5 XC
	8.65e-17	1.01e-15	1.46	0.0	A-PINENE + O3 = #.7 HO. + #.081 RO2-R. + #.321 RO2-N. + #1.375 R2O2. + #.298 RCO-O2. + #.051 CO + #.339 HCHO + #.218 RCHO + #.345 ACET + #.002 GLY + #.081 BACL + #.3 RCO-OH + #3.875 XC
	6.16e-12	1.19e-12	-0.97	0.0	A-PINENE + NO3 = #.75 NO2 + #.25 RO2-N. + #.75 R2O2. + #.75 RCHO + #6.25 XC + #.25 XN
	3.20e-11	3.20e-11	0.00	0.0	A-PINENE + O3P = PROD2 + #4 XC
b-Pinene [PM]	7.88e-11	2.38e-11	-0.71	0.0	B-PINENE + HO. = #.75 RO2-R. + #.25 RO2-N. + #.5 R2O2. + #.75 HCHO + #.75 PROD2 + #3.25 XC
	1.50e-17	1.01e-15	2.49	0.0	B-PINENE + O3 = #.34 HO. + #.09 HO2. + #.05 RO2-N. + #.2 R2O2. + #.2 RCO-O2. + #.375 CO + #.1 CO2 + #.25 HCHO + #.75 PROD2 + #.28 HCOOH + #3.595 XC
	2.51e-12	2.51e-12	0.00	0.0	B-PINENE + NO3 = #.75 RO2-R. + #.25 RO2-N. + #.75 R2O2. + #.75 RNO3 + #4 XC + #.25 XN
	2.70e-11	2.70e-11	0.00	0.0	B-PINENE + O3P = #.4 RCHO + #.6 PROD2 + #5.2 XC
d-Limonene [PM]	1.71e-10	3.19e-11	-0.99	0.0	D-LIMONE + HO. = #.75 RO2-R. + #.25 RO2-N. + #.5 R2O2. + #.75 RCHO + #6.25 XC
	2.00e-16	3.71e-15	1.73	0.0	D-LIMONE + O3 = #.7 HO. + #.161 RO2-N. + #.539 R2O2. + #.482 CCO-O2. + #.058 RCO-O2. + #.058 HCHO + #.482 RCHO + #.3 RCO-OH + #5.492 XC
	1.22e-11	1.22e-11	0.00	0.0	D-LIMONE + NO3 = #.75 NO2 + #.25 RO2-N. + #.75 R2O2. + #.75 RCHO + #6.25 XC + #.25 XN
	7.20e-11	7.20e-11	0.00	0.0	D-LIMONE + O3P = PROD2 + #4 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Sabinene [PM]	1.17e-10	2.19e-11	-0.99	0.0	SABINENE + HO. = #.75 RO2-R. + #.25 RO2-N. + #.5 R2O2. + #.75 HCHO + #.75 PROD2 + #3.25 XC
	8.60e-17	1.01e-15	1.46	0.0	SABINENE + O3 = #.34 HO. + #.09 HO2. + #.05 RO2-N. + #.2 R2O2. + #.2 RCO-O2. + #.375 CO + #.1 CO2 + #.25 HCHO + #.75 PROD2 + #.28 HCOOH + #3.595 XC
	1.00e-11	1.00e-11	0.00	0.0	SABINENE + NO3 = #.75 RO2-R. + #.25 RO2-N. + #.75 R2O2. + #.75 RNO3 + #4 XC + #.25 XN
	1.69e-11	1.69e-11	0.00	0.0	SABINENE + O3P = #.4 RCHO + #.6 PROD2 + #5.2 XC
Styrene [PM]	5.80e-11	5.80e-11	0.00	0.0	STYRENE + HO. = #.87 RO2-R. + #.13 RO2-N. + #.87 HCHO + #.87 BALD + #.26 XC
	1.71e-17	1.71e-17	0.00	0.0	STYRENE + O3 = #.4 HCHO + #.6 BALD + #.6 HCOOH + #.4 RCO-OH + #1.6 XC
	1.51e-13	1.51e-13	0.00	0.0	STYRENE + NO3 = #.22 NO2 + #.65 RO2-R. + #.13 RO2-N. + #.22 R2O2. + #.22 HCHO + #.22 BALD + #.65 RNO3 + #1.56 XC + #.13 XN
	1.76e-11	1.76e-11	0.00	0.0	STYRENE + O3P = PROD2 + #2 XC
Benzene [PM]	1.23e-12	2.47e-12	0.41	0.0	BENZENE + HO. = #.236 HO2. + #.764 RO2-R. + #.207 GLY + #.236 PHEN + #.764 DCB1 + #1.114 XC
Toluene [PM]	5.95e-12	1.81e-12	-0.71	0.0	TOLUENE + HO. = #.234 HO2. + #.758 RO2-R. + #.008 RO2-N. + #.116 GLY + #.135 MGLY + #.234 CRES + #.085 BALD + #.46 DCB1 + #.156 DCB2 + #.057 DCB3 + #1.178 XC
Ethyl Benzene [PM]	7.10e-12	7.10e-12	0.00	0.0	C2-BENZ + HO. = #.19 HO2. + #.786 RO2-R. + #.024 RO2-N. + #.239 PROD2 + #.094 GLY + #.109 MGLY + #.19 CRES + #.498 DCB1 + #.049 DCB3 + #2.338 XC
Isopropyl Benzene (cumene) [PM]	6.50e-12	6.50e-12	0.00	0.0	I-C3-BEN + HO. = #.19 HO2. + #.786 RO2-R. + #.024 RO2-N. + #.239 PROD2 + #.094 GLY + #.109 MGLY + #.19 CRES + #.498 DCB1 + #.049 DCB3 + #3.338 XC
n-Propyl Benzene [PM]	6.00e-12	6.00e-12	0.00	0.0	N-C3-BEN + HO. = #.19 HO2. + #.786 RO2-R. + #.024 RO2-N. + #.239 PROD2 + #.094 GLY + #.109 MGLY + #.19 CRES + #.498 DCB1 + #.049 DCB3 + #3.338 XC
s-Butyl Benzene [PM]	6.00e-12	6.00e-12	0.00	0.0	S-C4-BEN + HO. = #.19 HO2. + #.786 RO2-R. + #.024 RO2-N. + #.239 PROD2 + #.094 GLY + #.109 MGLY + #.19 CRES + #.498 DCB1 + #.049 DCB3 + #4.338 XC
m-Xylene [PM]	2.36e-11	2.36e-11	0.00	0.0	M-XYLENE + HO. = #.21 HO2. + #.782 RO2-R. + #.008 RO2-N. + #.107 GLY + #.335 MGLY + #.21 CRES + #.037 BALD + #.347 DCB1 + #.29 DCB2 + #.108 DCB3 + #1.628 XC
o-Xylene [PM]	1.37e-11	1.37e-11	0.00	0.0	O-XYLENE + HO. = #.161 HO2. + #.831 RO2-R. + #.008 RO2-N. + #.084 GLY + #.238 MGLY + #.139 BACL + #.161 CRES + #.054 BALD + #.572 DCB1 + #.06 DCB2 + #.145 DCB3 + #1.697 XC
p-Xylene [PM]	1.43e-11	1.43e-11	0.00	0.0	P-XYLENE + HO. = #.188 HO2. + #.804 RO2-R. + #.008 RO2-N. + #.195 GLY + #.112 MGLY + #.188 CRES + #.083 BALD + #.709 DCB1 + #.012 DCB3 + #2.432 XC
1,2,3-Trimethyl Benzene [PM]	3.27e-11	3.27e-11	0.00	0.0	123-TMB + HO. = #.186 HO2. + #.804 RO2-R. + #.01 RO2-N. + #.065 GLY + #.166 MGLY + #.383 BACL + #.186 CRES + #.044 BALD + #.533 DCB1 + #.077 DCB2 + #.149 DCB3 + #1.904 XC
1,2,4-Trimethyl Benzene [PM]	3.25e-11	3.25e-11	0.00	0.0	124-TMB + HO. = #.186 HO2. + #.804 RO2-R. + #.01 RO2-N. + #.063 GLY + #.364 MGLY + #.079 BACL + #.186 CRES + #.044 BALD + #.733 DCB1 + #.027 DCB3 + #2.73 XC
1,3,5-Trimethyl Benzene [PM]	5.75e-11	5.75e-11	0.00	0.0	135-TMB + HO. = #.186 HO2. + #.804 RO2-R. + #.01 RO2-N. + #.621 MGLY + #.186 CRES + #.025 BALD + #.569 DCB1 + #.097 DCB2 + #.114 DCB3 + #2.273 XC
Naphthalene [PM]	2.16e-11	1.07e-12	-1.78	0.0	NAPHTHAL + HO. = #.236 HO2. + #.215 RO2-R. + #.07 RO2-N. + #.479 RCO-O2. + #.084 GLY + #.236 PHEN + #.117 DCB1 + #.049 DCB2 + #.049 DCB3 + #5.601 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Tetralin [PM]	3.43e-11	3.43e-11	0.00	0.0	TETRALIN + HO. = #.6 HO2. + #.108 RO2-R. + #.129 RO2-N. + #.163 RCO-O2. + #.084 GLY + #.6 PHEN + #.016 DCB1 + #.046 DCB2 + #.046 DCB3 + #4.446 XC
Methyl Naphthalenes [PM]	5.20e-11	5.20e-11	0.00	0.0	ME-NAPH + HO. = #.236 HO2. + #.155 RO2-R. + #.07 RO2-N. + #.539 RCO-O2. + #.084 GLY + #.038 MGLY + #.236 CRES + #.003 DCB1 + #.076 DCB2 + #.076 DCB3 + #6.259 XC
2,3-Dimethyl Naphth. [PM]	7.68e-11	7.68e-11	0.00	0.0	23-DMN + HO. = #.236 HO2. + #.094 RO2-R. + #.07 RO2-N. + #.6 RCO-O2. + #.084 GLY + #.076 MGLY + #.236 CRES + #.103 DCB2 + #.103 DCB3 + #6.709 XC
Acetylene	8.97e-13	9.40e-12	1.39		ACETYLEN + HO. = #.603 HO. + #.297 HO2. + #.1 RO2-R. + #.393 CO + #.096 HCHO + #.607 GLY + #.297 HCOOH + #-0 XC
	7.80e-21	2.00e-14	8.74		ACETYLEN + O3 = #.5 HO. + #1.5 HO2. + #1.5 CO + #.5 CO2
Methyl Acetylene	5.90e-12	5.90e-12			ME-ACTYL + HO. = #.67 HO. + #.33 CCO-O2. + #.67 MGLY + #.33 HCOOH + #-0 XC
	1.43e-20	1.00e-14	7.97		ME-ACTYL + O3 = HO. + R2O2. + RCO-O2. + HCHO + #-1 XC
2-Butyne	2.74e-11	1.00e-11	-0.60		2-BUTYNE + HO. = #.67 HO. + #.33 CCO-O2. + #.67 BACL + #.33 CCO-OH + #-0 XC
	1.97e-20	1.00e-14	7.78		2-BUTYNE + O3 = HO. + #.039 RO2-N. + #.961 R2O2. + #.961 RCO-O2. + #.961 HCHO + #-0.079 XC
Ethyl Acetylene [LP]	8.00e-12	8.00e-12			ET-ACTYL + HO. = #.67 HO. + #.33 RCO-O2. + #.67 MGLY + #.33 HCOOH + #.67 XC
	1.97e-20	1.00e-14	7.78		ET-ACTYL + O3 = HO. + #.039 RO2-N. + #.961 R2O2. + #.961 RCO-O2. + #.961 CCHO + #-1.039 XC
Ethyl Acetylene [AP]	8.00e-12	8.00e-12			ET-ACTYL + HO. = #.67 HO. + #.33 RCO-O2. + #.33 HCOOH + #.67 XC + #.67 PRD1
	1.97e-20	1.00e-14	7.78		ET-ACTYL + O3 = HO. + #.039 RO2-N. + #.961 R2O2. + #.961 RCO-O2. + #.961 CCHO + #-1.039 XC
	1.30e-11	1.30e-11			PRD1 + HO. = #.035 RO2-R. + #.004 RO2-N. + #.057 R2O2. + #.961 RCO-O2. + #.001 HCHO + #.052 CCHO + #.035 MGLY + #-0.117 XC
	2.53e-15	2.53e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=MGLY_ADJ			PRD1 + HV = HO2. + RCO-O2. + CO + #-1 XC
Methanol	9.27e-13	3.10e-12	0.72		MEOH + HO. = HO2. + HCHO
Ethanol	3.31e-12	5.56e-13	-1.06		ETOH + HO. = #.95 HO2. + #.05 RO2-R. + #.081 HCHO + #.96 CCHO + #-0 XC
Isopropyl Alcohol	5.39e-12	6.49e-13	-1.25		I-C3-OH + HO. = #.953 HO2. + #.046 RO2-R. + #.001 RO2-N. + #.046 HCHO + #.046 CCHO + #.953 ACET + #-0.003 XC
n-Propyl Alcohol [LP]	5.53e-12	5.53e-12			N-C3-OH + HO. = #.759 HO2. + #.238 RO2-R. + #.003 RO2-N. + #.208 HCHO + #.207 CCHO + #.79 RCHO + #-0.009 XC
n-Propyl Alcohol [AP]	5.53e-12	5.53e-12			N-C3-OH + HO. = #.759 HO2. + #.238 RO2-R. + #.003 RO2-N. + #.208 HCHO + #.207 CCHO + #.759 RCHO + #-0.009 XC + #.031 PRD1
	2.43e-11	2.43e-11			PRD1 + HO. = #.166 HO2. + #.036 RO2-R. + #.797 RCO-O2. + #.035 CO + #.001 HCHO + #.035 CCHO + #.166 RCHO + #.001 GLY + #-0 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + CO + #1.611 HCHO + #.195 CCHO
Isobutyl Alcohol [LP]	6.91e-12	6.91e-12			I-C4-OH + HO. = #.56 HO2. + #.403 RO2-R. + #.037 RO2-N. + #.393 HCHO + #.036 CCHO + #.607 RCHO + #.319 ACET + #.531 XC
Isobutyl Alcohol [AP]	6.91e-12	6.91e-12			I-C4-OH + HO. = #.56 HO2. + #.403 RO2-R. + #.037 RO2-N. + #.393 HCHO + #.036 CCHO + #.319 ACET + #.531 XC + #.607 PRD1
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
n-Butyl Alcohol [LP]	8.57e-12	8.57e-12			N-C4-OH + HO. = #.517 HO2. + #.47 RO2-R. + #.013 RO2-N. + #.308 HCHO + #.08 CCHO + #.827 RCHO + #.093 PROD2 + #.414 XC
n-Butyl Alcohol [AP]	8.57e-12	8.57e-12			N-C4-OH + HO. = #.517 HO2. + #.47 RO2-R. + #.013 RO2-N. + #.308 HCHO + #.08 CCHO + #.2 RCHO + #.414 XC + #.627 PRD1 + #.093 PRD2
	2.34e-11	2.34e-11			PRD1 + HO. = #.011 HO2. + #.088 RO2-R. + #.007 RO2-N. + #.014 R2O2. + #.894 RCO-O2. + #.051 CO + #.017 HCHO + #.014 CCHO + #.084 RCHO + #.001 GLY + #-0.077 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.999 HO2. + #.982 RO2-R. + #.019 RO2-N. + CO + #.002 HCHO + #.98 RCHO + #-1.056 XC
	1.38e-11	1.38e-11			PRD2 + HO. = #.875 HO2. + #.061 RO2-R. + #.003 RO2-N. + #.061 CCO-O2. + #.061 CCHO + #.936 RCHO + #2.931 XC
		PF=KETONE QY = 1.0e-1			PRD2 + HV = RO2-R. + CCO-O2. + #1.611 HCHO + #.195 CCHO + #2 XC
s-Butyl Alcohol	9.95e-12	9.95e-12			S-C4-OH + HO. = #.829 HO2. + #.165 RO2-R. + #.006 RO2-N. + #.016 HCHO + #.238 CCHO + #.033 RCHO + #.843 MEK + #.005 XC
t-Butyl Alcohol	1.14e-12	3.86e-13	-0.64		T-C4-OH + HO. = #.693 RO2-R. + #.052 RO2-N. + #.254 TBU-O. + #.693 HCHO + #.693 ACET + #.15 XC
Cyclopentanol [LP]	1.07e-11	1.07e-11			CC5-OH + HO. = #.399 HO2. + #.562 RO2-R. + #.039 RO2-N. + #.004 CO + #.101 HCHO + #.33 RCHO + #.631 MEK + #1.147 XC
Cyclopentanol [AP]	1.07e-11	1.07e-11			CC5-OH + HO. = #.399 HO2. + #.562 RO2-R. + #.039 RO2-N. + #.004 CO + #.101 HCHO + #.631 MEK + #1.147 XC + #.33 PRD1
	4.11e-11	4.11e-11			PRD1 + HO. = #.04 RO2-R. + #.007 RO2-N. + #.031 R2O2. + #.953 RCO-O2. + #.036 CO + #.014 HCHO + #.04 RCHO + #.001 GLY + #-0.072 XC
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.405 HO2. + #.976 RO2-R. + #.024 RO2-N. + #.595 RCO-O2. + CO + #.381 RCHO + #-1.073 XC
2-Pentanol [LP]	1.18e-11	1.18e-11			2-C5OH + HO. = #.643 HO2. + #.335 RO2-R. + #.022 RO2-N. + #.034 HCHO + #.146 CCHO + #.141 RCHO + #.73 MEK + #.093 PROD2 + #.642 XC
2-Pentanol [AP]	1.18e-11	1.18e-11			2-C5OH + HO. = #.643 HO2. + #.335 RO2-R. + #.022 RO2-N. + #.034 HCHO + #.146 CCHO + #.141 RCHO + #.73 MEK + #.642 XC + #.093 PRD1
	2.83e-11	2.83e-11			PRD1 + HO. = #.753 HO2. + #.188 RO2-R. + #.013 RO2-N. + #.042 CCO-O2. + #.003 RCO-O2. + #.145 HCHO + #.4 RCHO + #.584 MEK + #2.147 XC
		PF=KETONE QY = 3.0e-2			PRD1 + HV = RO2-R. + #.004 R2O2. + CCO-O2. + #.6 HCHO + #.59 CCHO + #.406 RCHO + XC
3-Pentanol	1.22e-11	1.22e-11			3-C5OH + HO. = #.765 HO2. + #.22 RO2-R. + #.015 RO2-N. + #.174 CCHO + #.195 RCHO + #.79 MEK + #.817 XC
Pentyl Alcohol [LP]	1.11e-11	1.11e-11			C5OH + HO. = #.375 HO2. + #.59 RO2-R. + #.035 RO2-N. + #.262 HCHO + #.027 CCHO + #.881 RCHO + #.084 PROD2 + #1.326 XC
Pentyl Alcohol [AP]	1.11e-11	1.11e-11			C5OH + HO. = #.375 HO2. + #.59 RO2-R. + #.035 RO2-N. + #.262 HCHO + #.027 CCHO + #.066 RCHO + #1.326 XC + #.815 PRD1 + #.084 PRD2
	2.76e-11	2.76e-11			PRD1 + HO. = #.053 HO2. + #.086 RO2-R. + #.013 RO2-N. + #.052 R2O2. + #.848 RCO-O2. + #.041 CO + #.01 HCHO + #.024 CCHO + #.134 RCHO + #.002 MGLY + #-0.131 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.387 HO2. + #1.553 RO2-R. + #.06 RO2-N. + CO + #.94 RCHO + #-1.179 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.49e-11	1.49e-11			PRD2 + HO. = #.752 HO2. + #.136 RO2-R. + #.009 RO2-N. + #.103 RCO-O2. + #.103 CCHO + #.888 RCHO + #2.766 XC
	PF=KETONE QY = 5.0e-2				PRD2 + HV = RO2-R. + RCO-O2. + #1.611 HCHO + #.195 CCHO + XC
Cyclohexanol [LP]	1.74e-11	1.74e-11			CC6-OH + HO. = #.439 HO2. + #.506 RO2-R. + #.055 RO2-N. + #.04 HCHO + #.246 RCHO + #.705 PROD2 + #.664 XC
Cyclohexanol [AP]	1.74e-11	1.74e-11			CC6-OH + HO. = #.439 HO2. + #.506 RO2-R. + #.055 RO2-N. + #.04 HCHO + #.664 XC + #.705 PRD1 + #.246 PRD2
	1.05e-11	1.05e-11			PRD1 + HO. = #.091 HO2. + #.38 RO2-R. + #.155 RO2-N. + #.604 R2O2. + #.374 RCO-O2. + #.056 HCHO + #.2 RCHO + #.274 PROD2 + #1.644 XC
	PF=KETONE QY = 4.5e-2				PRD1 + HV = #5.911 XC
	4.27e-11	4.27e-11			PRD2 + HO. = #.035 RO2-R. + #.016 RO2-N. + #.07 R2O2. + #.949 RCO-O2. + #.02 CO + #.005 HCHO + #.023 RCHO + #.013 MGLY + #-0.076 XC
	7.60e-15	7.60e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.069 HO2. + #1.617 RO2-R. + #.106 RO2-N. + #.207 RCO-O2. + #1.049 CO + #.687 RCHO + #-1.369 XC
1-Hexanol [LP]	1.25e-11	1.25e-11			1-C6OH + HO. = #.108 HO2. + #.814 RO2-R. + #.078 RO2-N. + #.098 HCHO + #.002 CCHO + #.675 RCHO + #.253 PROD2 + #1.885 XC
1-Hexanol [AP]	1.25e-11	1.25e-11			1-C6OH + HO. = #.108 HO2. + #.814 RO2-R. + #.078 RO2-N. + #.098 HCHO + #.002 CCHO + #.006 RCHO + #1.885 XC + #.669 PRD1 + #.253 PRD2
	2.68e-11	2.68e-11			PRD1 + HO. = #.065 HO2. + #.112 RO2-R. + #.032 RO2-N. + #.11 R2O2. + #.792 RCO-O2. + #.016 CO + #.003 HCHO + #.006 CCHO + #.177 RCHO + #.015 MGLY + #-0.172 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.085 HO2. + #1.795 RO2-R. + #.119 RO2-N. + CO + #.018 CCHO + #.881 RCHO + #-1.394 XC
	2.04e-11	2.04e-11			PRD2 + HO. = #.648 HO2. + #.261 RO2-R. + #.028 RO2-N. + #.015 CCO-O2. + #.047 RCO-O2. + #.073 HCHO + #.152 CCHO + #.591 RCHO + #.323 PROD2 + #.037 MGLY + #1.459 XC
	PF=KETONE QY = 1.0e-2				PRD2 + HV = #.256 HO2. + #.729 RO2-R. + #.015 RO2-N. + #.378 CCO-O2. + #.622 RCO-O2. + #.846 HCHO + #.071 CCHO + #.363 RCHO + #1.211 XC
2-Hexanol [LP]	1.21e-11	1.21e-11			2-C6OH + HO. = #.543 HO2. + #.415 RO2-R. + #.043 RO2-N. + #.032 HCHO + #.13 CCHO + #.15 RCHO + #.808 PROD2 + #.155 XC
2-Hexanol [AP]	1.21e-11	1.21e-11			2-C6OH + HO. = #.543 HO2. + #.415 RO2-R. + #.043 RO2-N. + #.032 HCHO + #.13 CCHO + #.017 RCHO + #.155 XC + #.133 PRD1 + #.808 PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	1.17e-11	1.17e-11			PRD2 + HO. = #.125 HO2. + #.392 RO2-R. + #.088 RO2-N. + #.825 R2O2. + #.381 CCO-O2. + #.014 RCO-O2. + #.276 HCHO + #.195 CCHO + #.581 RCHO + #.175 MEK + #.142 PROD2 + #.704 XC
	PF=KETONE QY = 4.4e-2				PRD2 + HV = #.935 RO2-R. + #.065 RO2-N. + #.707 R2O2. + #.932 CCO-O2. + #.068 RCO-O2. + #.06 HCHO + #.06 CCHO + #.876 RCHO + #.738 XC
1-Heptanol [LP]	1.37e-11	1.37e-11			1-C7OH + HO. = #.862 RO2-R. + #.138 RO2-N. + #.025 R2O2. + #.054 HCHO + #.547 RCHO + #.315 PROD2 + #2.587 XC
1-Heptanol [AP]	1.37e-11	1.37e-11			1-C7OH + HO. = #.862 RO2-R. + #.138 RO2-N. + #.025 R2O2. + #.054 HCHO + #2.587 XC + #.547 PRD1 + #.315 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.76e-11	2.76e-11			PRD1 + HO. = #.055 HO2. + #.143 RO2-R. + #.055 RO2-N. + #.143 R2O2. + #.747 RCO-O2. + #.009 CO + #.201 RCHO + #.016 MGLY + #-0.234 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.095 HO2. + #1.725 RO2-R. + #.18 RO2-N. + CO + #.839 RCHO + #-1.599 XC
	2.30e-11	2.30e-11			PRD2 + HO. = #.641 HO2. + #.259 RO2-R. + #.04 RO2-N. + #.009 CCO-O2. + #.051 RCO-O2. + #.005 HCHO + #.131 CCHO + #.526 RCHO + #.438 PROD2 + #.021 MGLY + #1.052 XC
1-Octanol [LP]	2.02e-11	2.02e-11			1-C8-OH + HO. = #.771 RO2-R. + #.229 RO2-N. + #.32 R2O2. + #.054 HCHO + #.387 RCHO + #.384 PROD2 + #3.108 XC
1-Octanol [AP]	2.02e-11	2.02e-11			1-C8-OH + HO. = #.771 RO2-R. + #.229 RO2-N. + #.32 R2O2. + #.054 HCHO + #3.108 XC + #.387 PRD1 + #.384 PRD2
	2.97e-11	2.97e-11			PRD1 + HO. = #.068 HO2. + #.171 RO2-R. + #.075 RO2-N. + #.147 R2O2. + #.686 RCO-O2. + #.007 CO + #.248 RCHO + #.014 MGLY + #-0.303 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.13 HO2. + #1.627 RO2-R. + #.243 RO2-N. + CO + #.777 RCHO + #-1.786 XC
	2.49e-11	2.49e-11			PRD2 + HO. = #.545 HO2. + #.319 RO2-R. + #.066 RO2-N. + #.004 CCO-O2. + #.065 RCO-O2. + #.011 HCHO + #.071 CCHO + #.544 RCHO + #.45 PROD2 + #.016 MGLY + #.86 XC
2-Ethyl-1-Hexanol [LP]	1.33e-11	1.33e-11			2-ETC6OH + HO. = #.006 HO2. + #.841 RO2-R. + #.153 RO2-N. + #.339 HCHO + #.04 CCHO + #.604 RCHO + #.327 PROD2 + #2.884 XC
2-Ethyl-1-Hexanol [AP]	1.33e-11	1.33e-11			2-ETC6OH + HO. = #.006 HO2. + #.841 RO2-R. + #.153 RO2-N. + #.339 HCHO + #.04 CCHO + #.083 RCHO + #2.884 XC + #.521 PRD1 + #.327 PRD2
	2.79e-11	2.79e-11			PRD1 + HO. = #.049 HO2. + #.155 RO2-R. + #.057 RO2-N. + #.115 R2O2. + #.739 RCO-O2. + #.096 CO + #.003 HCHO + #.025 CCHO + #.168 RCHO + #.057 PROD2 + #.009 MGLY + #-0.58 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.324 HO2. + #1.434 RO2-R. + #.242 RO2-N. + CO + #.002 HCHO + #.116 CCHO + #.292 RCHO + #.468 PROD2 + #-3.365 XC
	9.16e-12	9.16e-12			PRD2 + HO. = #.095 HO2. + #.513 RO2-R. + #.134 RO2-N. + #.523 R2O2. + #.01 CCO-O2. + #.248 RCO-O2. + #.074 HCHO + #.294 CCHO + #.51 RCHO + #.19 MEK + #.131 PROD2 + #.692 XC
		PF=KETONE QY = 1.6e-2			PRD2 + HV = #.931 RO2-R. + #.069 RO2-N. + #.759 R2O2. + RCO-O2. + #.931 RCHO + #-0.208 XC
2-Octanol [LP]	2.52e-11	2.52e-11			2-C8-OH + HO. = #.062 HO2. + #.775 RO2-R. + #.163 RO2-N. + #.008 HCHO + #.183 CCHO + #.198 RCHO + #.64 PROD2 + #2.219 XC
2-Octanol [AP]	2.52e-11	2.52e-11			2-C8-OH + HO. = #.062 HO2. + #.775 RO2-R. + #.163 RO2-N. + #.008 HCHO + #.183 CCHO + #2.219 XC + #.64 PRD1 + #.198 PRD2
	1.79e-11	1.79e-11			PRD1 + HO. = #.256 HO2. + #.418 RO2-R. + #.197 RO2-N. + #.532 R2O2. + #.119 CCO-O2. + #.01 RCO-O2. + #.008 HCHO + #.017 CCHO + #.3 RCHO + #.574 PROD2 + #.164 XC
		PF=KETONE QY = 5.8e-3			PRD1 + HV = #.814 RO2-R. + #.186 RO2-N. + #.902 R2O2. + CCO-O2. + #.814 RCHO + #.443 XC
	2.82e-11	2.82e-11			PRD2 + HO. = #.123 HO2. + #.117 RO2-R. + #.028 RO2-N. + #.086 R2O2. + #.731 RCO-O2. + #.012 CO + #.001 HCHO + #.007 CCHO + #.247 RCHO + #.016 MGLY + #-0.181 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.034 CCHO + #.874 RCHO + #-1.445 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
3-Octanol [LP]	3.14e-11	3.14e-11			3-C8-OH + HO. = #.225 HO2. + #.641 RO2-R. + #.134 RO2-N. + #.142 CCHO + #.355 RCHO + #.609 PROD2 + #2.19 XC
3-Octanol [AP]	3.14e-11	3.14e-11			3-C8-OH + HO. = #.225 HO2. + #.641 RO2-R. + #.134 RO2-N. + #.142 CCHO + #.098 RCHO + #2.19 XC + #.609 PRD1 + #.257 PRD2
	1.28e-11	1.28e-11			PRD1 + HO. = #.164 HO2. + #.443 RO2-R. + #.193 RO2-N. + #.57 R2O2. + #.003 CCO-O2. + #.196 RCO-O2. + #.013 HCHO + #.079 CCHO + #.487 RCHO + #.405 PROD2 + #.181 XC
	PF=KETONE QY = 7.2e-3				PRD1 + HV = #.874 RO2-R. + #.126 RO2-N. + #.935 R2O2. + RCO-O2. + #.874 RCHO + #-0.377 XC
	2.83e-11	2.83e-11			PRD2 + HO. = #.068 HO2. + #.11 RO2-R. + #.024 RO2-N. + #.082 R2O2. + #.798 RCO-O2. + #.023 CO + #.005 HCHO + #.008 CCHO + #.177 RCHO + #.002 GLY + #.011 MGLY + #-0.152 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.316 HO2. + #1.592 RO2-R. + #.091 RO2-N. + CO + #.179 HCHO + #.909 RCHO + #-1.452 XC
4-Octanol [LP]	2.87e-11	2.87e-11			4-C8-OH + HO. = #.161 HO2. + #.693 RO2-R. + #.145 RO2-N. + #.715 RCHO + #.497 PROD2 + #2.002 XC
4-Octanol [AP]	2.87e-11	2.87e-11			4-C8-OH + HO. = #.161 HO2. + #.693 RO2-R. + #.145 RO2-N. + #.18 RCHO + #2.002 XC + #.497 PRD1 + #.535 PRD2
	1.29e-11	1.29e-11			PRD1 + HO. = #.053 HO2. + #.487 RO2-R. + #.181 RO2-N. + #.535 R2O2. + #.279 RCO-O2. + #.102 HCHO + #.22 CCHO + #.389 RCHO + #.377 PROD2 + #.104 XC
	PF=KETONE QY = 7.9e-3				PRD1 + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #-0.06 XC
	2.61e-11	2.61e-11			PRD2 + HO. = #.079 HO2. + #.077 RO2-R. + #.008 RO2-N. + #.024 R2O2. + #.835 RCO-O2. + #.038 CO + #.01 HCHO + #.018 CCHO + #.145 RCHO + #.006 GLY + #.001 MGLY + #-0.088 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.848 HO2. + #1.121 RO2-R. + #.031 RO2-N. + CO + #.255 HCHO + #.117 CCHO + #.852 RCHO + #-1.232 XC
8-Methyl-1-Nonanol (Isodecyl Alcohol) [LP]	1.54e-11	1.54e-11			I-C10-OH + HO. = #.7 RO2-R. + #.3 RO2-N. + #.31 R2O2. + #.037 HCHO + #.395 RCHO + #.009 ACET + #.306 PROD2 + #5.121 XC
8-Methyl-1-Nonanol (Isodecyl Alcohol) [AP]	1.54e-11	1.54e-11			I-C10-OH + HO. = #.7 RO2-R. + #.3 RO2-N. + #.31 R2O2. + #.037 HCHO + #.009 ACET + #5.121 XC + #.395 PRD1 + #.306 PRD2
	3.14e-11	3.14e-11			PRD1 + HO. = #.024 HO2. + #.197 RO2-R. + #.139 RO2-N. + #.256 R2O2. + #.639 RCO-O2. + #.007 CO + #.225 RCHO + #.004 ACET + #.01 MGLY + #-0.475 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.069 HO2. + #1.537 RO2-R. + #.393 RO2-N. + CO + #.508 RCHO + #.106 PROD2 + #-2.521 XC
	2.68e-11	2.68e-11			PRD2 + HO. = #.343 HO2. + #.437 RO2-R. + #.122 RO2-N. + #.005 R2O2. + #.001 C-O2. + #.097 RCO-O2. + #.077 HCHO + #.052 CCHO + #.546 RCHO + #.101 ACET + #.354 PROD2 + #.01 MGLY + #.694 XC
Ethylene Glycol	1.47e-11	1.47e-11			ET-GLYCL + HO. = HO2. + #.067 HCHO + #.966 CCHO
Propylene Glycol [LP]	2.15e-11	2.15e-11			PR-GLYCL + HO. = #.987 HO2. + #.013 RO2-R. + #.039 HCHO + #.039 CCHO + #.315 RCHO + #.646 MEK + #-0.646 XC
Propylene Glycol [AP]	2.15e-11	2.15e-11			PR-GLYCL + HO. = #.987 HO2. + #.013 RO2-R. + #.039 HCHO + #.039 CCHO + #.646 MEK + #-0.646 XC + #.315 PRD1
	2.46e-11	2.46e-11			PRD1 + HO. = #.209 HO2. + #.791 RCO-O2. + #.209 MGLY + #-0 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + CCHO
1,2-Butandiol [LP]	1.59e-11	1.59e-11			12-C4OH2 + HO. = #.916 HO2. + #.081 RO2-R. + #.003 RO2-N. + #.022 HCHO + #.14 CCHO + #.285 RCHO + #.641 MEK + #.257 XC
1,2-Butandiol [AP]	1.59e-11	1.59e-11			12-C4OH2 + HO. = #.916 HO2. + #.081 RO2-R. + #.003 RO2-N. + #.022 HCHO + #.14 CCHO + #.022 RCHO + #.641 MEK + #.257 XC + #.264 PRD1
	2.69e-11	2.69e-11			PRD1 + HO. = #.234 HO2. + #.042 RO2-R. + #.002 RO2-N. + #.723 RCO-O2. + #.042 CCHO + #.042 GLY + #.234 MGLY + #-0.047 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + RCHO + #-1 XC
Glycerol [LP]	1.87e-11	1.87e-11			GLYCERL + HO. = HO2. + #.017 HCHO + #.017 CCHO + #.435 RCHO + #.548 PROD2 + #-1.645 XC
Glycerol [AP]	1.87e-11	1.87e-11			GLYCERL + HO. = HO2. + #.017 HCHO + #.017 CCHO + #-1.645 XC + #.435 PRD1 + #.548 PRD2
	2.98e-11	2.98e-11			PRD1 + HO. = #.347 HO2. + #.653 RCO-O2. + #.136 RCHO + #.211 MGLY + #-0 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + CCHO
	6.01e-12	6.01e-12			PRD2 + HO. = #.817 HO2. + #.183 RCO-O2. + #.183 HCHO + #.817 MGLY + #2.817 XC
		PF=KETONE QY = 1.0e-1			PRD2 + HV = HO2. + RCO-O2. + HCHO + #2 XC
1,2-Dihydroxy Hexane [LP]	1.87e-11	1.87e-11			C6-GLYCL + HO. = #.779 HO2. + #.2 RO2-R. + #.022 RO2-N. + #.069 CCHO + #.36 RCHO + #.618 PROD2 + #.943 XC
1,2-Dihydroxy Hexane [AP]	1.87e-11	1.87e-11			C6-GLYCL + HO. = #.779 HO2. + #.2 RO2-R. + #.022 RO2-N. + #.069 CCHO + #.943 XC + #.618 PRD1 + #.36 PRD2
	1.03e-11	1.03e-11			PRD1 + HO. = #.054 HO2. + #.68 RO2-R. + #.067 RO2-N. + #.113 R2O2. + #.199 RCO-O2. + #.108 HCHO + #.159 CCHO + #.288 RCHO + #.106 MEK + #.102 PROD2 + #.382 MGLY + #1.528 XC
		PF=KETONE QY = 1.9e-2			PRD1 + HV = HO2. + RCO-O2. + HCHO + #2 XC
	3.03e-11	3.03e-11			PRD2 + HO. = #.186 HO2. + #.105 RO2-R. + #.011 RO2-N. + #.003 R2O2. + #.699 RCO-O2. + #.01 CO + #.003 HCHO + #.003 CCHO + #.106 RCHO + #.026 GLY + #.188 MGLY + #-0.115 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #1.808 HO2. + #.188 RO2-R. + #.004 RO2-N. + CO + #.996 RCHO + #-1.012 XC
2-Methyl-2,4-Pentanediol [LP]	1.06e-11	1.06e-11			2M24C5OH + HO. = #.785 HO2. + #.195 RO2-R. + #.02 RO2-N. + #.046 HCHO + #.012 CCHO + #.141 RCHO + #.133 ACET + #.785 MEK + #.042 PROD2 + #1.595 XC
2-Methyl-2,4-Pentanediol [AP]	1.06e-11	1.06e-11			2M24C5OH + HO. = #.785 HO2. + #.195 RO2-R. + #.02 RO2-N. + #.046 HCHO + #.012 CCHO + #.133 ACET + #.785 MEK + #1.595 XC + #.042 PRD1 + #.141 PRD2
	5.51e-12	5.51e-12			PRD1 + HO. = #.633 HO2. + #.187 RO2-R. + #.02 RO2-N. + #.142 CCO-O2. + #.017 RCO-O2. + #.109 HCHO + #.871 RCHO + #.092 MEK + #2.454 XC
		PF=KETONE QY = 1.0e-2			PRD1 + HV = #.961 RO2-R. + #.039 RO2-N. + CCO-O2. + #.961 HCHO + #.961 MEK + #-1.039 XC
	2.46e-11	2.46e-11			PRD2 + HO. = #.209 HO2. + #.791 RCO-O2. + #.209 MGLY + #-0 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #2 HO2. + CO + CCHO
Dimethyl Ether	2.99e-12	1.04e-11	0.74		ME-O-ME + HO. = RO2-R. + #.079 HCHO + #.961 INERT + #.961 XC
Trimethylene Oxide [LP]	1.03e-11	1.03e-11			TME-OX + HO. = #.138 RO2-R. + #1.862 R2O2. + #.862 RCO-O2. + #.003 CO + #.006 HCHO + #.135 RCHO + #-0 XC
Trimethylene Oxide [AP]	1.03e-11	1.03e-11			TME-OX + HO. = #.138 RO2-R. + #1.862 R2O2. + #.862 RCO-O2. + #.003 CO + #.006 HCHO + #-0 XC + #.135 PRD1

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.99e-11	1.99e-11			PRD1 + HO. = #.031 RO2-R. + #.001 R2O2. + #.969 RCO-O2. + #.031 CO + #.001 HCOOH + #.03 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + #1.411 CO + #.071 CO2 + #.071 HCHO + #.411 HCOOH + #.518 XC
Tetrahydrofuran [LP]	1.61e-11	1.61e-11			THF + HO. = #.911 RO2-R. + #.079 RO2-N. + #1.032 R2O2. + #.009 RCO-O2. + #.049 CO + #.013 HCHO + #.861 RCHO + #.05 PROD2 + #.549 XC
Tetrahydrofuran [AP]	1.61e-11	1.61e-11			THF + HO. = #.911 RO2-R. + #.079 RO2-N. + #1.032 R2O2. + #.009 RCO-O2. + #.049 CO + #.013 HCHO + #.549 XC + #.861 PRD1 + #.05 PRD2
	2.11e-11	2.11e-11			PRD1 + HO. = #.036 RO2-R. + #.004 RO2-N. + #.051 R2O2. + #.961 RCO-O2. + #.029 CO + #.006 CO2 + #.036 RCHO + #.04 HCOOH + #-0.086 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.082 HO2. + RO2-R. + #.918 RCO-O2. + CO + #.082 RCHO + #-1 XC
	5.23e-12	5.23e-12			PRD2 + HO. = #.71 HO2. + #.199 RO2-R. + #.091 RCO-O2. + #.005 CO2 + #.13 HCHO + #.005 CCHO + #.77 RCHO + #.004 MEK + #.06 HCOOH + #3.066 XC
Diethyl Ether	1.33e-11	8.02e-13	-1.66		ET-O-ET + HO. = #.131 RO2-R. + #.04 RO2-N. + #.848 R2O2. + #.829 C-O2. + #.006 HCHO + #.168 CCHO + #.006 RCHO + #.858 MEK + #.01 PROD2 + #-0.924 XC
Dimethoxy methane [LP]	4.90e-12	4.90e-12			METHYLAL + HO. = RO2-R. + #.086 HCHO + #.639 PROD2 + #.359 INERT + #-1.282 XC
Dimethoxy methane [AP]	4.90e-12	4.90e-12			METHYLAL + HO. = RO2-R. + #.086 HCHO + #.359 INERT + #-1.282 XC + #.639 PRD1
	8.17e-12	8.17e-12			PRD1 + HO. = RO2-R. + #.003 CO + #.86 CO2 + #.007 HCHO + #.134 MEK + #.003 HCOOH + #3.728 XC
Alpha-Methyltetrahydrofuran [LP]	2.23e-11	2.52e-12	-1.29		AM-THF + HO. = #.817 RO2-R. + #.141 RO2-N. + #1.221 R2O2. + #.04 C-O2. + #.003 RCO-O2. + #.01 CO + #.025 HCHO + #.008 CCHO + #.847 RCHO + #.007 PROD2 + #1.472 XC
Alpha-Methyltetrahydrofuran [AP]	2.23e-11	2.52e-12	-1.29		AM-THF + HO. = #.817 RO2-R. + #.141 RO2-N. + #1.221 R2O2. + #.04 C-O2. + #.003 RCO-O2. + #.01 CO + #.025 HCHO + #.008 CCHO + #.007 PROD2 + #1.472 XC + #.847 PRD1
	2.32e-11	2.32e-11			PRD1 + HO. = #.034 HO2. + #.067 RO2-R. + #.008 RO2-N. + #.052 R2O2. + #.891 RCO-O2. + #.034 CO + #.007 CO2 + #.023 HCHO + #.1 RCHO + #.001 HCOOH + #.048 CCO-OH + #-0.184 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.675 HO2. + #.992 RO2-R. + #.038 RO2-N. + #.008 CCO-O2. + #.286 RCO-O2. + CO + #.001 CO2 + #.045 HCHO + #.001 CCHO + #.651 RCHO + #.015 HCOOH + #-1.138 XC
Tetrahydropyran [LP]	1.38e-11	1.38e-11			THP + HO. = #.824 RO2-R. + #.167 RO2-N. + #1.606 R2O2. + #.009 RCO-O2. + #.025 CO + #.026 HCHO + #.694 RCHO + #.13 PROD2 + #.001 GLY + #.008 HCOOH + #1.046 XC
Tetrahydropyran [AP]	1.38e-11	1.38e-11			THP + HO. = #.824 RO2-R. + #.167 RO2-N. + #1.606 R2O2. + #.009 RCO-O2. + #.025 CO + #.026 HCHO + #.001 GLY + #.008 HCOOH + #1.046 XC + #.694 PRD1 + #.13 PRD2
	2.89e-11	2.89e-11			PRD1 + HO. = #.233 HO2. + #.073 RO2-R. + #.005 RO2-N. + #.004 R2O2. + #.689 RCO-O2. + #.028 CO + #.306 RCHO + #-0.073 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.966 HO2. + #.98 RO2-R. + #.039 RO2-N. + #.014 RCO-O2. + CO + #.024 HCHO + #.942 RCHO + #-1.134 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.69e-11	1.69e-11			PRD2 + HO. = #.177 HO2. + #.467 RO2-R. + #.077 RO2-N. + #.685 R2O2. + #.28 RCO-O2. + #.001 CO2 + #.048 HCHO + #.001 CCHO + #.543 RCHO + #.001 MEK + #.067 PROD2 + #.015 HCOOH + #2.554 XC
	PF=KETONE QY = 3.8e-2				PRD2 + HV = #5 XC
Ethyl Isopropyl Ether	2.44e-11	2.44e-11			ET-O-IPR + HO. = #.246 RO2-R. + #.066 RO2-N. + #.701 R2O2. + #.688 C-O2. + #.008 HCHO + #.221 CCHO + #.002 RCHO + #.219 ACET + #.709 MEK + #.004 PROD2 + #-0.052 XC
Methyl n-Butyl Ether [LP]	1.48e-11	1.48e-11			MNBE + HO. = #.919 RO2-R. + #.081 RO2-N. + #.783 R2O2. + #.006 HCHO + #.038 CCHO + #.72 RCHO + #.068 MEK + #.131 PROD2 + #.693 INERT + #.521 XC
Methyl n-Butyl Ether [AP]	1.48e-11	1.48e-11			MNBE + HO. = #.919 RO2-R. + #.081 RO2-N. + #.783 R2O2. + #.006 HCHO + #.038 CCHO + #.673 RCHO + #.068 MEK + #.693 INERT + #.521 XC + #.047 PRD1 + #.131 PRD2
	2.62e-11	2.62e-11			PRD1 + HO. = #.262 RO2-R. + #.005 R2O2. + #.738 RCO-O2. + #.225 CO + #.004 HCHO + #.037 RCHO + #.223 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + CO + #.079 HCHO + #.961 XC
	1.95e-11	1.95e-11			PRD2 + HO. = #.092 RO2-R. + #.066 RO2-N. + #1.274 R2O2. + #.423 CCO-O2. + #.418 RCO-O2. + #.417 HCHO + #.043 CCHO + #.025 RCHO + #.08 MEK + #1.82 XC
	PF=KETONE QY = 5.0e-2				PRD2 + HV = RO2-R. + #.12 R2O2. + #.468 CCO-O2. + #.532 RCO-O2. + #.051 HCHO + #.001 CCHO + #.393 RCHO + #.072 PROD2 + #1.295 XC
Methyl t-Butyl Ether	2.94e-12	5.89e-13	-0.96	2.0	MTBE + HO. = #.743 RO2-R. + #.078 RO2-N. + #.381 R2O2. + #.162 C-O2. + #.016 TBU-O. + #.234 HCHO + #.024 ACET + #.719 MEK + #.007 PROD2 + #.155 INERT + #.939 XC
Di n-Propyl Ether [LP]	1.88e-11	1.18e-12	-1.64		PR-O-PR + HO. = #.894 RO2-R. + #.106 RO2-N. + #.961 R2O2. + #.873 CCHO + #.014 RCHO + #.795 MEK + #.085 PROD2 + #-0.116 XC
Di n-Propyl Ether [AP]	1.88e-11	1.18e-12	-1.64		PR-O-PR + HO. = #.894 RO2-R. + #.106 RO2-N. + #.961 R2O2. + #.873 CCHO + #.014 RCHO + #.795 MEK + #-0.116 XC + #.085 PRD1
	9.66e-12	9.66e-12			PRD1 + HO. = #.858 HO2. + #.12 RO2-R. + #.005 RO2-N. + #.017 RCO-O2. + #.017 HCHO + #.103 CCHO + #.017 RCHO + #.858 MEK + #2.11 XC
Ethyl n-Butyl Ether [LP]	2.13e-11	2.13e-11			ENBE + HO. = #.589 RO2-R. + #.116 RO2-N. + #.882 R2O2. + #.295 C-O2. + #.011 HCHO + #.086 CCHO + #.491 RCHO + #.721 MEK + #.104 PROD2 + #-0.154 XC
Ethyl n-Butyl Ether [AP]	2.13e-11	2.13e-11			ENBE + HO. = #.589 RO2-R. + #.116 RO2-N. + #.882 R2O2. + #.295 C-O2. + #.011 HCHO + #.086 CCHO + #.432 RCHO + #.721 MEK + #-0.154 XC + #.104 PRD1 + #.059 PRD2
	2.70e-11	2.70e-11			PRD1 + HO. = #.361 HO2. + #.107 RO2-R. + #.059 RO2-N. + #.848 R2O2. + #.074 C-O2. + #.393 CCO-O2. + #.006 RCO-O2. + #.38 HCHO + #.054 CCHO + #.107 RCHO + #.821 MEK + #.007 PROD2 + #.599 XC
	PF=KETONE QY = 1.1e-2				PRD1 + HV = #.531 RO2-R. + #.061 RO2-N. + #1.267 R2O2. + #.408 C-O2. + CCO-O2. + #.265 HCHO + #.196 CCHO + #.29 RCHO + #.484 PROD2 + #-1.208 XC
	2.57e-11	2.57e-11			PRD2 + HO. = #.157 HO2. + #.086 RO2-R. + #.004 RO2-N. + #.753 RCO-O2. + #.033 CO + #.053 HCHO + #.243 RCHO + #-0.097 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.987 HO2. + #1.013 RO2-R. + CO + #.033 HCHO + #.002 CCHO + #.987 RCHO + #-1 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Ethyl t-Butyl Ether	8.84e-12	8.84e-12			ETBE + HO. = #.143 RO2-R. + #.101 RO2-N. + #.81 R2O2. + #.644 C-O2. + #.112 TBU-O. + #.055 HCHO + #.127 CCHO + #.018 RCHO + #.016 ACET + #.644 MEK + #.109 INERT + #1.317 XC
Methyl t-Amyl Ether	7.91e-12	7.91e-12			MTAE + HO. = #.535 RO2-R. + #.13 RO2-N. + #1.076 R2O2. + #.335 C-O2. + #.219 HCHO + #.512 CCHO + #.028 RCHO + #.055 ACET + #.33 MEK + #.026 PROD2 + #.001 HCOOH + #.432 INERT + #1.488 XC
2-Butyl Tetra-hydrofuran [LP]	2.76e-11	2.76e-11			2BU-THF + HO. = #.642 RO2-R. + #.356 RO2-N. + #1.176 R2O2. + #.002 RCO-O2. + #.001 CO + #.034 HCHO + #.733 RCHO + #.001 MEK + #.003 PROD2 + #.002 HCOOH + #3.603 XC
2-Butyl Tetra-hydrofuran [AP]	2.76e-11	2.76e-11			2BU-THF + HO. = #.642 RO2-R. + #.356 RO2-N. + #1.176 R2O2. + #.002 RCO-O2. + #.001 CO + #.034 HCHO + #.026 RCHO + #.001 MEK + #.003 PROD2 + #.002 HCOOH + #3.603 XC + #.706 PRD1
	2.65e-11	2.65e-11			PRD1 + HO. = #.046 HO2. + #.118 RO2-R. + #.034 RO2-N. + #.081 R2O2. + #.801 RCO-O2. + #.027 CO + #.001 CO2 + #.002 HCHO + #.023 CCHO + #.18 RCHO + #.001 MEK + #.035 PROD2 + #.002 MGLY + #.005 BACL + #.006 HCOOH + #.002 RCO-OH + #-0.48 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.707 HO2. + #1.031 RO2-R. + #.129 RO2-N. + #.133 RCO-O2. + CO + #.007 HCHO + #.787 RCHO + #.001 PROD2 + #-1.554 XC
Di-Isobutyl Ether	2.60e-11	2.60e-11			IBU2-O + HO. = #.767 RO2-R. + #.233 RO2-N. + #.961 R2O2. + #.019 HCHO + #.006 RCHO + #.763 ACET + #.778 MEK + #.013 PROD2 + #1.083 XC
Di-n-butyl Ether [LP]	2.88e-11	2.88e-11			BU-O-BU + HO. = #.788 RO2-R. + #.212 RO2-N. + #.903 R2O2. + #.032 CCHO + #.737 RCHO + #.651 MEK + #.147 PROD2 + #.969 XC
Di-n-butyl Ether [AP]	2.88e-11	2.88e-11			BU-O-BU + HO. = #.788 RO2-R. + #.212 RO2-N. + #.903 R2O2. + #.032 CCHO + #.737 RCHO + #.651 MEK + #.969 XC + #.147 PRD1
	2.47e-11	2.47e-11			PRD1 + HO. = #.482 HO2. + #.189 RO2-R. + #.079 RO2-N. + #.567 R2O2. + #.243 CCO-O2. + #.008 RCO-O2. + #.236 HCHO + #.056 CCHO + #.182 RCHO + #.785 MEK + #.017 PROD2 + #.834 XC
Di-n-Pentyl Ether [LP]	3.47e-11	3.47e-11			C5-O-C5 + HO. = #.679 RO2-R. + #.321 RO2-N. + #1.291 R2O2. + #.007 CCHO + #.604 RCHO + #.704 PROD2 + #2.027 XC
Di-n-Pentyl Ether [AP]	3.47e-11	3.47e-11			C5-O-C5 + HO. = #.679 RO2-R. + #.321 RO2-N. + #1.291 R2O2. + #.007 CCHO + #.033 RCHO + #2.027 XC + #.704 PRD1 + #.571 PRD2
	8.31e-12	8.31e-12			PRD1 + HO. = #.035 HO2. + #.56 RO2-R. + #.147 RO2-N. + #.851 R2O2. + #.258 RCO-O2. + #.033 HCHO + #.021 CCHO + #.167 RCHO + #.569 PROD2 + #.012 HCOOH + #.337 XC
	2.52e-11	2.52e-11			PRD2 + HO. = #.122 HO2. + #.086 RO2-R. + #.004 RO2-N. + #.003 R2O2. + #.787 RCO-O2. + #.037 CO + #.045 HCHO + #.003 CCHO + #.205 RCHO + #-0.092 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + #-0 XC + XN PRD2 + HV = #.99 HO2. + #1.005 RO2-R. + #.004 RO2-N. + CO + #.026 HCHO + #.002 CCHO + #.986 RCHO + #-1.013 XC
2-Methoxy-ethanol [LP]	1.34e-11	4.50e-12	-0.65		MEO-ETOH + HO. = #.278 HO2. + #.722 RO2-R. + #.648 HCHO + #.307 RCHO + #.048 PROD2 + #.642 INERT + #.497 XC
2-Methoxy-ethanol [AP]	1.34e-11	4.50e-12	-0.65		MEO-ETOH + HO. = #.278 HO2. + #.722 RO2-R. + #.648 HCHO + #.642 INERT + #.497 XC + #.048 PRD1 + #.307 PRD2
	5.23e-12	5.23e-12			PRD1 + HO. = #.71 HO2. + #.199 RO2-R. + #.091 RCO-O2. + #.005 CO2 + #.13 HCHO + #.005 CCHO + #.77 RCHO + #.004 MEK + #.06 HCOOH + #3.066 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.88e-11	2.88e-11			PRD2 + HO. = #.05 HO2. + #.248 RO2-R. + #.004 R2O2. + #.702 RCO-O2. + #.214 CO + #.003 HCHO + #.084 RCHO + #.011 MEK + #.18 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + RO2-R. + CO + #.076 HCHO + #.092 MEK + #.004 HCOOH + #.684 XC
1-Methoxy-2-Propanol [LP]	2.00e-11	2.00e-11			MEOC3OH + HO. = #.39 HO2. + #.6 RO2-R. + #.01 RO2-N. + #.001 HCHO + #.571 CCHO + #.419 PROD2 + #.571 INERT + #-0.287 XC
1-Methoxy-2-Propanol [AP]	2.00e-11	2.00e-11			MEOC3OH + HO. = #.39 HO2. + #.6 RO2-R. + #.01 RO2-N. + #.001 HCHO + #.571 CCHO + #.571 INERT + #-0.287 XC + #.419 PRD1
	6.77e-12	6.77e-12			PRD1 + HO. = #.148 RO2-R. + #.039 RO2-N. + #.812 R2O2. + #.798 CCO-O2. + #.014 RCO-O2. + #.028 HCHO + #.148 MEK + #2.712 XC
		PF=KETONE QY = 1.0e-1			PRD1 + HV = RO2-R. + CCO-O2. + #.079 HCHO + #2.961 XC
2-Ethoxyethanol [LP]	1.87e-11	1.87e-11			ETO-ETOH + HO. = #.015 HO2. + #.792 RO2-R. + #.02 RO2-N. + #.173 C-O2. + #.549 HCHO + #.083 CCHO + #.268 RCHO + #.437 MEK + #.206 PROD2 + #-0.793 XC
2-Ethoxyethanol [AP]	1.87e-11	1.87e-11			ETO-ETOH + HO. = #.015 HO2. + #.792 RO2-R. + #.02 RO2-N. + #.173 C-O2. + #.549 HCHO + #.083 CCHO + #.437 MEK + #-0.793 XC + #.206 PRD1 + #.268 PRD2
	5.36e-12	5.36e-12			PRD1 + HO. = #.707 HO2. + #.214 RO2-R. + #.002 RO2-N. + #.077 RCO-O2. + #.004 CO2 + #.155 HCHO + #.004 CCHO + #.758 RCHO + #.003 MEK + #.05 HCOOH + #.001 CCO-OH + #3.095 XC
	4.75e-11	4.75e-11			PRD2 + HO. = #.207 HO2. + #.177 RO2-R. + #.012 RO2-N. + #.124 R2O2. + #.118 C-O2. + #.487 RCO-O2. + #.164 CO + #.024 HCHO + #.025 CCHO + #.336 RCHO + #.12 MEK + #.021 PROD2 + #.001 GLY + #-0.502 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.987 HO2. + RO2-R. + #.013 C-O2. + CO + #.046 HCHO + #.032 CCHO + #.668 MEK + #.286 PROD2 + #.013 HCOOH + #.001 CCO-OH + #-2.526 XC
2-Methoxy-1-Propanol [LP]	2.53e-11	2.53e-11			2MEOC3OH + HO. = #.161 HO2. + #.806 RO2-R. + #.033 RO2-N. + #.763 HCHO + #.001 CCHO + #.178 RCHO + #.027 PROD2 + #.761 INERT + #1.58 XC
2-Methoxy-1-Propanol [AP]	2.53e-11	2.53e-11			2MEOC3OH + HO. = #.161 HO2. + #.806 RO2-R. + #.033 RO2-N. + #.763 HCHO + #.001 CCHO + #.761 INERT + #1.58 XC + #.027 PRD1 + #.178 PRD2
	6.51e-12	6.51e-12			PRD1 + HO. = #.592 HO2. + #.348 RO2-R. + #.014 RO2-N. + #.003 CCO-O2. + #.043 RCO-O2. + #.008 CO2 + #.317 HCHO + #.621 RCHO + #.007 MEK + #.004 HCOOH + #3.248 XC
	3.26e-11	3.26e-11			PRD2 + HO. = #.388 RO2-R. + #.016 RO2-N. + #.004 R2O2. + #.596 RCO-O2. + #.359 CO + #.001 HCHO + #.001 CCHO + #.029 RCHO + #.308 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.216 HO2. + RO2-R. + #.784 C-O2. + CO + #.139 HCHO + #.139 CCHO + #-0.063 XC
1-Ethoxy-2-Propanol [LP]	2.62e-11	2.62e-11			ETOC3OH + HO. = #.163 HO2. + #.633 RO2-R. + #.044 RO2-N. + #.16 C-O2. + #.033 HCHO + #.415 CCHO + #.349 MEK + #.574 PROD2 + #-1.127 XC
1-Ethoxy-2-Propanol [AP]	2.62e-11	2.62e-11			ETOC3OH + HO. = #.163 HO2. + #.633 RO2-R. + #.044 RO2-N. + #.16 C-O2. + #.033 HCHO + #.415 CCHO + #.349 MEK + #-1.127 XC + #.574 PRD1
	1.93e-11	1.93e-11			PRD1 + HO. = #.356 HO2. + #.07 RO2-R. + #.04 RO2-N. + #.522 R2O2. + #.233 C-O2. + #.295 CCO-O2. + #.005 RCO-O2. + #.054 HCHO + #.078 CCHO + #.006 RCHO + #.853 MEK + #.017 PROD2 + #1.145 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=KETONE QY = 3.2e-2				PRD1 + HV = #.992 RO2-R. + #.008 R2O2. + #.008 C-O2. + CCO-O2. + #.046 HCHO + #.037 CCHO + #.772 MEK + #.182 PROD2 + #.008 HCOOH + #-0.317 XC
2-Propoxy-ethanol [LP]	2.47e-11	2.47e-11			2PROETOH + HO. = #.943 RO2-R. + #.057 RO2-N. + #.245 R2O2. + #.406 HCHO + #.369 CCHO + #.165 RCHO + #.368 MEK + #.41 PROD2 + #-0.912 XC
2-Propoxy-ethanol [AP]	2.47e-11	2.47e-11			2PROETOH + HO. = #.943 RO2-R. + #.057 RO2-N. + #.245 R2O2. + #.406 HCHO + #.369 CCHO + #.368 MEK + #-0.912 XC + #.41 PRD1 + #.165 PRD2
	5.64e-12	5.64e-12			PRD1 + HO. = #.724 HO2. + #.192 RO2-R. + #.084 RCO-O2. + #.005 CO2 + #.119 HCHO + #.014 CCHO + #.7 RCHO + #.083 MEK + #.054 HCOOH + #2.977 XC
	3.60e-11	3.60e-11			PRD2 + HO. = #.431 RO2-R. + #.032 RO2-N. + #.277 R2O2. + #.537 RCO-O2. + #.176 CO + #.251 CCHO + #.255 RCHO + #.153 MEK + #.023 PROD2 + #-0.997 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.92 HO2. + #1.037 RO2-R. + #.043 RO2-N. + CO + #.04 HCHO + #.04 RCHO + #.84 MEK + #.077 PROD2 + #-2.239 XC
3-Ethoxy-1-Propanol [LP]	2.20e-11	2.20e-11			3ETOC3OH + HO. = #.706 RO2-R. + #.055 RO2-N. + #.475 R2O2. + #.239 C-O2. + #.69 HCHO + #.127 CCHO + #.28 RCHO + #.393 MEK + #.271 PROD2 + #-0.551 XC
3-Ethoxy-1-Propanol [AP]	2.20e-11	2.20e-11			3ETOC3OH + HO. = #.706 RO2-R. + #.055 RO2-N. + #.475 R2O2. + #.239 C-O2. + #.69 HCHO + #.127 CCHO + #.393 MEK + #-0.551 XC + #.271 PRD1 + #.28 PRD2
	6.65e-12	6.65e-12			PRD1 + HO. = #.465 HO2. + #.356 RO2-R. + #.015 RO2-N. + #.164 RCO-O2. + #.012 CO2 + #.175 HCHO + #.816 RCHO + #.005 MEK + #.133 HCOOH + #2.631 XC
	3.44e-11	3.44e-11			PRD2 + HO. = #.029 HO2. + #.243 RO2-R. + #.024 RO2-N. + #.286 R2O2. + #.127 C-O2. + #.578 RCO-O2. + #.202 CO + #.153 HCHO + #.033 CCHO + #.2 RCHO + #.184 MEK + #.007 GLY + #.001 MGLY + #-0.776 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.362 HO2. + #1.339 RO2-R. + #.039 RO2-N. + #.17 R2O2. + #.26 C-O2. + CO + #.46 HCHO + #.168 CCHO + #.185 RCHO + #.178 MEK + #.309 PROD2 + #-2.411 XC
3-Methoxy-1-Butanol [LP]	2.36e-12	2.36e-12			3MEOC4OH + HO. = #.933 RO2-R. + #.055 RO2-N. + #.582 R2O2. + #.012 C-O2. + #1.171 HCHO + #.155 CCHO + #.19 RCHO + #.001 MEK + #.037 PROD2 + #.714 INERT + #1.664 XC
3-Methoxy-1-Butanol [AP]	2.36e-12	2.36e-12			3MEOC4OH + HO. = #.933 RO2-R. + #.055 RO2-N. + #.582 R2O2. + #.012 C-O2. + #1.171 HCHO + #.155 CCHO + #.001 MEK + #.714 INERT + #1.664 XC + #.037 PRD1 + #.19 PRD2
	7.93e-12	7.93e-12			PRD1 + HO. = #.456 HO2. + #.484 RO2-R. + #.032 RO2-N. + #.008 CCO-O2. + #.02 RCO-O2. + #.237 CO2 + #.165 HCHO + #.013 CCHO + #.685 RCHO + #.237 PROD2 + #.008 HCOOH + #1.801 XC
	3.95e-11	3.95e-11			PRD2 + HO. = #.471 RO2-R. + #.031 RO2-N. + #.367 R2O2. + #.004 C-O2. + #.493 RCO-O2. + #.43 CO + #.346 HCHO + #.047 RCHO + #.015 GLY + #-0.047 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.041 HO2. + #1.235 RO2-R. + #.033 RO2-N. + #.444 R2O2. + #.691 C-O2. + CO + #.814 HCHO + #.123 CCHO + #.074 RCHO + #.012 PROD2 + #-1.001 XC
Diethylene Glycol [LP]	2.75e-11	2.75e-11			DET-GLCL + HO. = #.293 HO2. + #.679 RO2-R. + #.028 RO2-N. + #.679 HCHO + #.293 RCHO + #.679 PROD2 + #-1.802 XC
Diethylene Glycol [AP]	2.75e-11	2.75e-11			DET-GLCL + HO. = #.293 HO2. + #.679 RO2-R. + #.028 RO2-N. + #.679 HCHO + #-1.802 XC + #.293 PRD1 + #.679 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.88e-11	3.88e-11			PRD1 + HO. = #.104 HO2. + #.383 RO2-R. + #.016 RO2-N. + #.497 RCO-O2. + #.146 CO + #.238 HCHO + #.342 RCHO + #.146 PROD2 + #-0.867 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + CO + #.075 HCHO + #.006 CCHO + #.37 RCHO + #.601 PROD2 + #-2.803 XC
	5.23e-12	5.23e-12			PRD2 + HO. = #.71 HO2. + #.199 RO2-R. + #.091 RCO-O2. + #.005 CO2 + #.13 HCHO + #.005 CCHO + #.77 RCHO + #.004 MEK + #.06 HCOOH + #3.066 XC
1-Propoxy-2-Propanol [LP]	2.91e-11	2.91e-11			PROXC3OH + HO. = #.927 RO2-R. + #.073 RO2-N. + #.047 R2O2. + #.635 CCHO + #.302 MEK + #.625 PROD2 + #-0.666 XC
1-Propoxy-2-Propanol [AP]	2.91e-11	2.91e-11			PROXC3OH + HO. = #.927 RO2-R. + #.073 RO2-N. + #.047 R2O2. + #.635 CCHO + #.302 MEK + #-0.666 XC + #.625 PRD1
	1.30e-11	1.30e-11			PRD1 + HO. = #.459 HO2. + #.314 RO2-R. + #.05 RO2-N. + #.434 R2O2. + #.168 CCO-O2. + #.009 RCO-O2. + #.009 HCHO + #.297 CCHO + #.013 RCHO + #.847 MEK + #.025 PROD2 + #1.097 XC
		PF=KETONE QY = 9.3e-3			PRD1 + HV = #.957 RO2-R. + #.043 RO2-N. + #.08 R2O2. + CCO-O2. + #.04 HCHO + #.04 RCHO + #.84 MEK + #.077 PROD2 + #-0.239 XC
2-Butoxyethanol [LP]	2.57e-11	2.57e-11			BUO-ETOH + HO. = #.888 RO2-R. + #.112 RO2-N. + #.133 R2O2. + #.55 HCHO + #.013 CCHO + #.318 RCHO + #.508 MEK + #.26 PROD2 + #.211 XC
2-Butoxyethanol [AP]	2.57e-11	2.57e-11			BUO-ETOH + HO. = #.888 RO2-R. + #.112 RO2-N. + #.133 R2O2. + #.55 HCHO + #.013 CCHO + #.193 RCHO + #.508 MEK + #.211 XC + #.26 PRD1 + #.125 PRD2
	6.20e-12	6.20e-12			PRD1 + HO. = #.72 HO2. + #.197 RO2-R. + #.002 RO2-N. + #.081 RCO-O2. + #.004 CO2 + #.113 HCHO + #.016 CCHO + #.693 RCHO + #.108 MEK + #.052 HCOOH + #2.916 XC
	3.74e-11	3.74e-11			PRD2 + HO. = #.428 RO2-R. + #.055 RO2-N. + #.283 R2O2. + #.517 RCO-O2. + #.176 CO + #.012 CCHO + #.486 RCHO + #.142 MEK + #.034 PROD2 + #-1.312 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.867 HO2. + #1.06 RO2-R. + #.073 RO2-N. + CO + #.038 HCHO + #.037 RCHO + #.794 MEK + #.096 PROD2 + #-2.339 XC
3 methoxy -3 methyl-Butanol [LP]	7.10e-12	7.10e-12			3MOMC4OH + HO. = #.127 HO2. + #.655 RO2-R. + #.054 RO2-N. + #.164 C-O2. + #.11 HCHO + #.202 CCHO + #.599 RCHO + #.026 ACET + #.141 PROD2 + #.001 HCOOH + #.18 INERT + #2.1 XC
3 methoxy -3 methyl-Butanol [AP]	7.10e-12	7.10e-12			3MOMC4OH + HO. = #.127 HO2. + #.655 RO2-R. + #.054 RO2-N. + #.164 C-O2. + #.11 HCHO + #.202 CCHO + #.026 ACET + #.001 HCOOH + #.18 INERT + #2.1 XC + #.141 PRD1 + #.599 PRD2
	5.95e-12	5.95e-12			PRD1 + HO. = #.457 HO2. + #.503 RO2-R. + #.04 RO2-N. + #.21 CO2 + #.018 HCHO + #.209 CCHO + #.749 RCHO + #.201 ACET + #.009 PROD2 + #2.205 XC
	2.18e-11	2.18e-11			PRD2 + HO. = #.007 HO2. + #.071 RO2-R. + #.013 RO2-N. + #.083 R2O2. + #.025 C-O2. + #.884 RCO-O2. + #.02 CO + #.031 HCHO + #.06 RCHO + #.004 ACET + #.002 PROD2 + #.031 GLY + #-0.111 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.003 HO2. + #1.155 RO2-R. + #.106 RO2-N. + #.669 R2O2. + #.735 C-O2. + CO + #1.088 HCHO + #.111 ACET + #-1.578 XC
2-(2-Methoxy-ethoxy) Ethanol [LP]	3.41e-11	3.41e-11			MOEOETOH + HO. = #.941 RO2-R. + #.059 RO2-N. + #.452 R2O2. + #.307 HCHO + #.001 CCHO + #.216 RCHO + #.019 MEK + #.717 PROD2 + #.001 HCOOH + #.518 INERT + #-1.211 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
2-(2-Methoxy-ethoxy) Ethanol [AP]	3.41e-11	3.41e-11			MOEOETOH + HO. = #.941 RO2-R. + #.059 RO2-N. + #.452 R2O2. + #.307 HCHO + #.001 CCHO + #.019 MEK + #.001 HCOOH + #.518 INERT + #-1.211 XC + #.717 PRD1 + #.216 PRD2
	7.67e-12	7.67e-12			PRD1 + HO. = #.445 HO2. + #.45 RO2-R. + #.015 RO2-N. + #.324 R2O2. + #.09 RCO-O2. + #.118 CO + #.026 CO2 + #.103 HCHO + #.003 CCHO + #.485 RCHO + #.035 MEK + #.004 PROD2 + #.181 HCOOH + #3.071 XC
	4.85e-11	4.85e-11			PRD2 + HO. = #.235 HO2. + #.334 RO2-R. + #.021 RO2-N. + #.245 R2O2. + #.41 RCO-O2. + #.121 CO + #.018 HCHO + #.447 RCHO + #.059 MEK + #.066 PROD2 + #-0.682 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.452 HO2. + #1.512 RO2-R. + #.036 RO2-N. + #.155 R2O2. + CO + #.044 HCHO + #.006 RCHO + #.757 MEK + #.165 PROD2 + #.036 HCOOH + #-2.671 XC
1-tert-Butoxy-2-Propanol [LP]	1.87e-11	1.87e-11			PG-1TB-E + HO. = #.407 HO2. + #.497 RO2-R. + #.077 RO2-N. + #.019 C-O2. + #.025 HCHO + #.452 CCHO + #.001 ACET + #.451 MEK + #.471 PROD2 + #.956 XC
1-tert-Butoxy-2-Propanol [AP]	1.87e-11	1.87e-11			PG-1TB-E + HO. = #.407 HO2. + #.497 RO2-R. + #.077 RO2-N. + #.019 C-O2. + #.025 HCHO + #.452 CCHO + #.001 ACET + #.451 MEK + #.956 XC + #.471 PRD1
	6.47e-12	6.47e-12			PRD1 + HO. = #.142 RO2-N. + #.927 R2O2. + #.059 C-O2. + #.786 CCO-O2. + #.014 RCO-O2. + #.086 HCHO + #.003 ACET + #.841 MEK + #.018 XC
		PF=KETONE QY = 1.0e-2			PRD1 + HV = #.9 RO2-R. + #.071 RO2-N. + #.049 R2O2. + #.009 C-O2. + CCO-O2. + #.021 TBU-O. + #.03 HCHO + #.899 MEK + #.009 PROD2 + #-0.178 XC
2-tert-Butoxy-1-Propanol [LP]	2.46e-11	2.46e-11			PG-2TB-E + HO. = #.132 HO2. + #.738 RO2-R. + #.115 RO2-N. + #.015 C-O2. + #.722 HCHO + #.166 RCHO + #.015 PROD2 + #.704 INERT + #4.279 XC
2-tert-Butoxy-1-Propanol [AP]	2.46e-11	2.46e-11			PG-2TB-E + HO. = #.132 HO2. + #.738 RO2-R. + #.115 RO2-N. + #.015 C-O2. + #.722 HCHO + #.015 PROD2 + #.704 INERT + #4.279 XC + #.166 PRD1
	3.20e-11	3.20e-11			PRD1 + HO. = #.329 RO2-R. + #.055 RO2-N. + #.026 R2O2. + #.012 C-O2. + #.604 RCO-O2. + #.329 CO + #.014 HCHO + #.001 CCHO + #.012 RCHO + #.001 ACET + #.136 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.216 HO2. + #.902 RO2-R. + #.098 RO2-N. + #.662 C-O2. + #.122 TBU-O. + CO + #.122 CCHO + #.662 MEK + #-2.623 XC
n-Butoxy-2-Propanol [LP]	3.05e-11	3.05e-11			BUOC3OH + HO. = #.89 RO2-R. + #.11 RO2-N. + #.064 R2O2. + #.333 CCHO + #.273 RCHO + #.276 MEK + #.618 PROD2 + #.041 XC
n-Butoxy-2-Propanol [AP]	3.05e-11	3.05e-11			BUOC3OH + HO. = #.89 RO2-R. + #.11 RO2-N. + #.064 R2O2. + #.333 CCHO + #.273 RCHO + #.276 MEK + #.041 XC + #.618 PRD1
	1.39e-11	1.39e-11			PRD1 + HO. = #.449 HO2. + #.303 RO2-R. + #.076 RO2-N. + #.428 R2O2. + #.163 CCO-O2. + #.009 RCO-O2. + #.008 HCHO + #.065 CCHO + #.234 RCHO + #.801 MEK + #.05 PROD2 + #.794 XC
		PF=KETONE QY = 4.7e-3			PRD1 + HV = #.927 RO2-R. + #.073 RO2-N. + #.133 R2O2. + CCO-O2. + #.038 HCHO + #.037 RCHO + #.794 MEK + #.096 PROD2 + #-0.339 XC
2-(2-Ethoxy-ethoxy) EtOH [LP]	5.08e-11	5.08e-11			CARBITOL + HO. = #.803 RO2-R. + #.117 RO2-N. + #.538 R2O2. + #.08 C-O2. + #.249 HCHO + #.027 CCHO + #.177 RCHO + #.405 MEK + #.757 PROD2 + #.003 HCOOH + #-1.781 XC
2-(2-Ethoxy-ethoxy) EtOH [AP]	5.08e-11	5.08e-11			CARBITOL + HO. = #.803 RO2-R. + #.117 RO2-N. + #.538 R2O2. + #.08 C-O2. + #.249 HCHO + #.027 CCHO + #.405 MEK + #.003 HCOOH + #-1.781 XC + #.757 PRD1 + #.177 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	1.10e-11	1.10e-11			PRD1 + HO. = #.456 HO2. + #.353 RO2-R. + #.025 RO2-N. + #.28 R2O2. + #.087 C-O2. + #.002 CCO-O2. + #.077 RCO-O2. + #.07 CO + #.016 CO2 + #.124 HCHO + #.021 CCHO + #.438 RCHO + #.263 MEK + #.05 PROD2 + #.111 HCOOH + #2.273 XC
	5.22e-11	5.22e-11			PRD2 + HO. = #.227 HO2. + #.32 RO2-R. + #.038 RO2-N. + #.297 R2O2. + #.036 C-O2. + #.379 RCO-O2. + #.116 CO + #.013 HCHO + #.012 CCHO + #.467 RCHO + #.232 MEK + #.089 PROD2 + #.001 HCOOH + #-1.415 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.437 HO2. + #1.5 RO2-R. + #.06 RO2-N. + #.139 R2O2. + #.003 C-O2. + CO + #.045 HCHO + #.002 CCHO + #.002 RCHO + #1.065 MEK + #.168 PROD2 + #.035 HCOOH + #-3.721 XC
Dipropylene Glycol [LP]	3.64e-11	3.64e-11			DPR-GLCL + HO. = #.464 HO2. + #.484 RO2-R. + #.052 RO2-N. + #.484 CCHO + #.948 PROD2 + #-0.968 XC
Dipropylene Glycol [AP]	3.64e-11	3.64e-11			DPR-GLCL + HO. = #.464 HO2. + #.484 RO2-R. + #.052 RO2-N. + #.484 CCHO + #-0.968 XC + #.948 PRD1
	1.68e-11	1.68e-11			PRD1 + HO. = #.5 HO2. + #.349 RO2-R. + #.034 RO2-N. + #.109 CCO-O2. + #.009 RCO-O2. + #.009 HCHO + #.231 CCHO + #.009 RCHO + #.616 MEK + #.28 PROD2 + #.86 XC
		PF=KETONE QY = 4.9e-3			PRD1 + HV = #.984 RO2-R. + #.016 RO2-N. + CCO-O2. + #.041 HCHO + #.021 CCHO + #.963 PROD2 + #-1.959 XC
2-Hexyloxy-ethanol [LP]	2.89e-11	2.89e-11			EGHE + HO. = #.788 RO2-R. + #.212 RO2-N. + #.566 R2O2. + #.282 HCHO + #.001 CCHO + #.389 RCHO + #.68 PROD2 + #1.195 XC
2-Hexyloxy-ethanol [AP]	2.89e-11	2.89e-11			EGHE + HO. = #.788 RO2-R. + #.212 RO2-N. + #.566 R2O2. + #.282 HCHO + #.001 CCHO + #.002 RCHO + #1.195 XC + #.68 PRD1 + #.387 PRD2
	8.85e-12	8.85e-12			PRD1 + HO. = #.348 HO2. + #.466 RO2-R. + #.12 RO2-N. + #.385 R2O2. + #.001 CCO-O2. + #.065 RCO-O2. + #.002 CO2 + #.08 HCHO + #.008 CCHO + #.41 RCHO + #.002 MEK + #.375 PROD2 + #.031 HCOOH + #1.405 XC
	3.40e-11	3.40e-11			PRD2 + HO. = #.17 HO2. + #.193 RO2-R. + #.055 RO2-N. + #.193 R2O2. + #.582 RCO-O2. + #.063 CO + #.028 CCHO + #.392 RCHO + #.047 PROD2 + #.001 MGLY + #-0.657 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.442 HO2. + #1.453 RO2-R. + #.105 RO2-N. + CO + #.013 HCHO + #.585 RCHO + #.31 PROD2 + #-2.258 XC
2-(2-Propoxy-ethoxy) ethanol [LP]	4.38e-11	4.38e-11			DGPE + HO. = #.866 RO2-R. + #.134 RO2-N. + #.535 R2O2. + #.214 HCHO + #.192 CCHO + #.177 RCHO + #.351 MEK + #.732 PROD2 + #-0.725 XC
2-(2-Propoxy-ethoxy) ethanol [AP]	4.38e-11	4.38e-11			DGPE + HO. = #.866 RO2-R. + #.134 RO2-N. + #.535 R2O2. + #.214 HCHO + #.192 CCHO + #.008 RCHO + #.351 MEK + #-0.725 XC + #.732 PRD1 + #.17 PRD2
	1.47e-11	1.47e-11			PRD1 + HO. = #.346 HO2. + #.561 RO2-R. + #.042 RO2-N. + #.315 R2O2. + #.051 RCO-O2. + #.086 CO + #.018 CO2 + #.175 HCHO + #.12 CCHO + #.378 RCHO + #.346 MEK + #.12 PROD2 + #.118 HCOOH + #1.553 XC
	5.38e-11	5.38e-11			PRD2 + HO. = #.236 HO2. + #.343 RO2-R. + #.053 RO2-N. + #.28 R2O2. + #.368 RCO-O2. + #.105 CO + #.011 HCHO + #.082 CCHO + #.481 RCHO + #.202 MEK + #.064 PROD2 + #-1.338 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.455 HO2. + #1.458 RO2-R. + #.086 RO2-N. + #.103 R2O2. + CO + #.042 HCHO + #.006 CCHO + #.001 RCHO + #1.019 MEK + #.159 PROD2 + #.034 HCOOH + #-3.635 XC
Dipropylene Glycol Methyl Ether [LP]	4.88e-11	4.88e-11			DPRGOME + HO. = #.785 RO2-R. + #.125 RO2-N. + #.475 R2O2. + #.09 C-O2. + #.047 HCHO + #.209 CCHO + #.014 MEK + #.856 PROD2 + #.001 HCOOH + #.511 INERT + #-0.01 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Dipropylene Glycol Methyl Ether [AP]	4.88e-11	4.88e-11			DPRGOME + HO. = #.785 RO2-R. + #.125 RO2-N. + #.475 R2O2. + #.09 C-O2. + #.047 HCHO + #.209 CCHO + #.014 MEK + #.001 HCOOH + #.511 INERT + #-0.01 XC + #.856 PRD1
	1.88e-11	1.88e-11			PRD1 + HO. = #.488 HO2. + #.26 RO2-R. + #.051 RO2-N. + #.494 R2O2. + #.033 C-O2. + #.163 CCO-O2. + #.005 RCO-O2. + #.032 CO2 + #.025 HCHO + #.101 CCHO + #.009 RCHO + #.654 MEK + #.055 PROD2 + #.125 HCOOH + #1.6 XC
	PF=KETONE QY = 1.0e-3				PRD1 + HV = #.957 RO2-R. + #.043 R2O2. + #.043 C-O2. + CCO-O2. + #.046 HCHO + #.954 PROD2 + #.043 HCOOH + #.003 CCO-OH + #-1.863 XC
2-(2-Butoxy-ethoxy)-EtOH [LP]	4.52e-11	4.52e-11			C8-CELSV + HO. = #.82 RO2-R. + #.18 RO2-N. + #.53 R2O2. + #.198 HCHO + #.01 CCHO + #.345 RCHO + #.317 MEK + #.708 PROD2 + #.149 XC
2-(2-Butox-yethoxy)-EtOH [AP]	4.52e-11	4.52e-11			C8-CELSV + HO. = #.82 RO2-R. + #.18 RO2-N. + #.53 R2O2. + #.198 HCHO + #.01 CCHO + #.174 RCHO + #.317 MEK + #.149 XC + #.708 PRD1 + #.171 PRD2
	1.50e-11	1.50e-11			PRD1 + HO. = #.353 HO2. + #.542 RO2-R. + #.054 RO2-N. + #.298 R2O2. + #.05 RCO-O2. + #.081 CO + #.017 CO2 + #.172 HCHO + #.011 CCHO + #.487 RCHO + #.321 MEK + #.126 PROD2 + #.113 HCOOH + #1.451 XC
	5.46e-11	5.46e-11			PRD2 + HO. = #.236 HO2. + #.329 RO2-R. + #.072 RO2-N. + #.278 R2O2. + #.363 RCO-O2. + #.101 CO + #.01 HCHO + #.004 CCHO + #.549 RCHO + #.188 MEK + #.065 PROD2 + #-1.432 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.456 HO2. + #1.426 RO2-R. + #.118 RO2-N. + #.064 R2O2. + CO + #.04 HCHO + #.006 RCHO + #.971 MEK + #.152 PROD2 + #.033 HCOOH + #-3.593 XC
2-[2-(2-Methoxyethoxy) ethoxy] ethanol [LP]	5.32e-11	5.32e-11			TGME + HO. = #.846 RO2-R. + #.154 RO2-N. + #.967 R2O2. + #.196 HCHO + #.001 CCHO + #.136 RCHO + #.191 MEK + #.922 PROD2 + #.009 HCOOH + #.403 INERT + #-1.232 XC
2-[2-(2-Methoxyethoxy) ethoxy] ethanol [AP]	5.32e-11	5.32e-11			TGME + HO. = #.846 RO2-R. + #.154 RO2-N. + #.967 R2O2. + #.196 HCHO + #.001 CCHO + #.191 MEK + #.009 HCOOH + #.403 INERT + #-1.232 XC + #.922 PRD1 + #.136 PRD2
	1.55e-11	1.55e-11			PRD1 + HO. = #.268 HO2. + #.628 RO2-R. + #.041 RO2-N. + #.412 R2O2. + #.063 RCO-O2. + #.123 CO + #.025 CO2 + #.169 HCHO + #.002 CCHO + #.331 RCHO + #.202 MEK + #.147 PROD2 + #.166 HCOOH + #1.928 XC
	5.92e-11	5.92e-11			PRD2 + HO. = #.225 HO2. + #.371 RO2-R. + #.067 RO2-N. + #.493 R2O2. + #.336 RCO-O2. + #.097 CO + #.018 HCHO + #.505 RCHO + #.138 MEK + #.14 PROD2 + #.004 HCOOH + #-1.622 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.434 HO2. + #1.476 RO2-R. + #.09 RO2-N. + #.107 R2O2. + CO + #.042 HCHO + #.001 RCHO + #.711 MEK + #.475 PROD2 + #.034 HCOOH + #-4.317 XC
2-(2-Ethyl-hexyloxy) ethanol [LP]	3.24e-11	3.24e-11			EGEHE + HO. = #.669 RO2-R. + #.331 RO2-N. + #.622 R2O2. + #.259 HCHO + #.046 CCHO + #.181 RCHO + #.792 PROD2 + #2.367 XC
2-(2-Ethyl-hexyloxy) ethanol [AP]	3.24e-11	3.24e-11			EGEHE + HO. = #.669 RO2-R. + #.331 RO2-N. + #.622 R2O2. + #.259 HCHO + #.046 CCHO + #.001 RCHO + #2.367 XC + #.792 PRD1 + #.18 PRD2
	1.14e-11	1.14e-11			PRD1 + HO. = #.372 HO2. + #.387 RO2-R. + #.148 RO2-N. + #.319 R2O2. + #.002 CCO-O2. + #.091 RCO-O2. + #.002 CO2 + #.074 HCHO + #.103 CCHO + #.427 RCHO + #.004 MEK + #.362 PROD2 + #.024 HCOOH + #1.012 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=KETONE QY = 2.2e-3				PRD1 + HV = #.93 RO2-R. + #.07 RO2-N. + #.785 R2O2. + RCO-O2. + #.93 RCHO + #-0.211 XC
	3.95e-11	3.95e-11			PRD2 + HO. = #.283 RO2-R. + #.179 RO2-N. + #.439 R2O2. + #.538 RCO-O2. + #.107 CO + #.003 HCHO + #.03 CCHO + #.261 RCHO + #.197 PROD2 + #-1.826 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.699 HO2. + #1.074 RO2-R. + #.227 RO2-N. + CO + #.022 HCHO + #.014 CCHO + #.217 RCHO + #.011 MEK + #.556 PROD2 + #-3.443 XC
2-[2-(2-Ethoxy-ethoxy) ethoxy] ethanol [LP]	6.00e-11	6.00e-11			TGEE + HO. = #.75 RO2-R. + #.199 RO2-N. + #.94 R2O2. + #.052 C-O2. + #.164 HCHO + #.018 CCHO + #.121 RCHO + #.486 MEK + #.905 PROD2 + #.009 HCOOH + #-1.189 XC
2-[2-(2-Ethoxy-ethoxy) ethoxy] ethanol [AP]	6.00e-11	6.00e-11			TGEE + HO. = #.75 RO2-R. + #.199 RO2-N. + #.94 R2O2. + #.052 C-O2. + #.164 HCHO + #.018 CCHO + #.486 MEK + #.009 HCOOH + #-1.189 XC + #.905 PRD1 + #.121 PRD2
	1.91e-11	1.91e-11			PRD1 + HO. = #.277 HO2. + #.537 RO2-R. + #.056 RO2-N. + #.403 R2O2. + #.072 C-O2. + #.001 CCO-O2. + #.057 RCO-O2. + #.089 CO + #.018 CO2 + #.165 HCHO + #.018 CCHO + #.312 RCHO + #.393 MEK + #.195 PROD2 + #.119 HCOOH + #1.117 XC
	6.30e-11	6.30e-11			PRD2 + HO. = #.227 HO2. + #.34 RO2-R. + #.089 RO2-N. + #.483 R2O2. + #.024 C-O2. + #.32 RCO-O2. + #.091 CO + #.014 HCHO + #.008 CCHO + #.507 RCHO + #.279 MEK + #.14 PROD2 + #.004 HCOOH + #-2.118 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.437 HO2. + #1.441 RO2-R. + #.122 RO2-N. + #.066 R2O2. + CO + #.04 HCHO + #.001 RCHO + #.693 MEK + #.44 PROD2 + #.033 HCOOH + #-4.222 XC
2-(2-Hexyloxy-ethoxy) ethanol [LP]	4.81e-11	4.81e-11			DGHE + HO. = #.724 RO2-R. + #.276 RO2-N. + #.65 R2O2. + #.172 HCHO + #.002 CCHO + #.285 RCHO + #.902 PROD2 + #1.902 XC
2-(2-Hexyloxy-ethoxy) ethanol [AP]	4.81e-11	4.81e-11			DGHE + HO. = #.724 RO2-R. + #.276 RO2-N. + #.65 R2O2. + #.172 HCHO + #.002 CCHO + #.001 RCHO + #1.902 XC + #.902 PRD1 + #.284 PRD2
	1.31e-11	1.31e-11			PRD1 + HO. = #.215 HO2. + #.597 RO2-R. + #.143 RO2-N. + #.532 R2O2. + #.045 RCO-O2. + #.05 CO + #.011 CO2 + #.121 HCHO + #.002 CCHO + #.334 RCHO + #.125 MEK + #.379 PROD2 + #.075 HCOOH + #.866 XC
	4.41e-11	4.41e-11			PRD2 + HO. = #.242 HO2. + #.201 RO2-R. + #.068 RO2-N. + #.19 R2O2. + #.489 RCO-O2. + #.062 CO + #.005 HCHO + #.021 CCHO + #.44 RCHO + #.024 MEK + #.095 PROD2 + #.001 MGLY + #-0.971 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.32 HO2. + #1.546 RO2-R. + #.134 RO2-N. + CO + #.02 HCHO + #.439 RCHO + #.334 MEK + #.213 PROD2 + #.016 HCOOH + #-2.769 XC
2-[2-(2-Propoxyethoxy) ethoxy] ethanol [LP]	6.30e-11	6.30e-11			TGPE + HO. = #.766 RO2-R. + #.234 RO2-N. + #.885 R2O2. + #.147 HCHO + #.124 CCHO + #.114 RCHO + #.428 MEK + #.854 PROD2 + #.007 HCOOH + #.015 XC
2-[2-(2-Propoxyethoxy) ethoxy] ethanol [AP]	6.30e-11	6.30e-11			TGPE + HO. = #.766 RO2-R. + #.234 RO2-N. + #.885 R2O2. + #.147 HCHO + #.124 CCHO + #.005 RCHO + #.428 MEK + #.007 HCOOH + #.015 XC + #.854 PRD1 + #.109 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.27e-11	2.27e-11			PRD1 + HO. = #.235 HO2. + #.643 RO2-R. + #.079 RO2-N. + #.435 R2O2. + #.043 RCO-O2. + #.084 CO + #.017 CO2 + #.167 HCHO + #.111 CCHO + #.313 RCHO + #.382 MEK + #.257 PROD2 + #.111 HCOOH + #.638 XC
	6.52e-11	6.52e-11			PRD2 + HO. = #.214 HO2. + #.365 RO2-R. + #.11 RO2-N. + #.478 R2O2. + #.311 RCO-O2. + #.086 CO + #.012 HCHO + #.061 CCHO + #.507 RCHO + #.259 MEK + #.125 PROD2 + #.003 HCOOH + #-2.127 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + #-0 XC + XN PRD2 + HV = #.412 HO2. + #1.427 RO2-R. + #.161 RO2-N. + #.028 R2O2. + CO + #.038 HCHO + #.001 RCHO + #.656 MEK + #.427 PROD2 + #.031 HCOOH + #-4.225 XC
2-[2-(2-Butoxy-ethoxy) ethoxy] ethanol [LP]	6.44e-11	6.44e-11			TGBE + HO. = #.729 RO2-R. + #.271 RO2-N. + #.861 R2O2. + #.139 HCHO + #.006 CCHO + #.225 RCHO + #.394 MEK + #.83 PROD2 + #.006 HCOOH + #.992 XC
2-[2-(2-Butoxy-ethoxy) ethoxy] ethanol [AP]	6.44e-11	6.44e-11			TGBE + HO. = #.729 RO2-R. + #.271 RO2-N. + #.861 R2O2. + #.139 HCHO + #.006 CCHO + #.114 RCHO + #.394 MEK + #.006 HCOOH + #.992 XC + #.83 PRD1 + #.11 PRD2
	2.30e-11	2.30e-11			PRD1 + HO. = #.239 HO2. + #.625 RO2-R. + #.094 RO2-N. + #.42 R2O2. + #.043 RCO-O2. + #.081 CO + #.016 CO2 + #.167 HCHO + #.007 CCHO + #.412 RCHO + #.356 MEK + #.262 PROD2 + #.107 HCOOH + #.55 XC
	6.62e-11	6.62e-11			PRD2 + HO. = #.21 HO2. + #.353 RO2-R. + #.13 RO2-N. + #.472 R2O2. + #.307 RCO-O2. + #.084 CO + #.012 HCHO + #.003 CCHO + #.557 RCHO + #.244 MEK + #.124 PROD2 + #.003 HCOOH + #-2.196 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.412 HO2. + #1.397 RO2-R. + #.191 RO2-N. + CO + #.037 HCHO + #.001 RCHO + #.631 MEK + #.405 PROD2 + #.03 HCOOH + #-4.168 XC
Tripropylene Glycol Monomethyl Ether [LP]	7.83e-11	7.83e-11			TPRGOME + HO. = #.572 RO2-R. + #.26 RO2-N. + #.993 R2O2. + #.169 C-O2. + #.029 HCHO + #.144 CCHO + #.098 MEK + #.946 PROD2 + #.021 HCOOH + #.402 INERT + #1.467 XC
Tripropylene Glycol Monomethyl Ether [AP]	7.83e-11	7.83e-11			TPRGOME + HO. = #.572 RO2-R. + #.26 RO2-N. + #.993 R2O2. + #.169 C-O2. + #.029 HCHO + #.144 CCHO + #.098 MEK + #.021 HCOOH + #.402 INERT + #1.467 XC + #.946 PRD1
	2.81e-11	2.81e-11			PRD1 + HO. = #.295 HO2. + #.416 RO2-R. + #.107 RO2-N. + #.587 R2O2. + #.043 C-O2. + #.132 CCO-O2. + #.007 RCO-O2. + #.04 CO + #.029 CO2 + #.017 HCHO + #.121 CCHO + #.006 RCHO + #.448 MEK + #.273 PROD2 + #.13 HCOOH + #.035 CCO-OH + #.658 XC
2,5,8,11-Tetraoxatridecan-13-ol [LP]	7.24e-11	7.24e-11			TETRAGME + HO. = #.746 RO2-R. + #.254 RO2-N. + #1.1 R2O2. + #.14 HCHO + #.001 CCHO + #.097 RCHO + #.234 MEK + #1.003 PROD2 + #.011 HCOOH + #.273 INERT + #-0.194 XC
2,5,8,11-Tetraoxatridecan-13-ol [AP]	7.24e-11	7.24e-11			TETRAGME + HO. = #.746 RO2-R. + #.254 RO2-N. + #1.1 R2O2. + #.14 HCHO + #.001 CCHO + #.234 MEK + #.011 HCOOH + #.273 INERT + #-0.194 XC + #1.003 PRD1 + #.097 PRD2
	2.37e-11	2.37e-11			PRD1 + HO. = #.168 HO2. + #.707 RO2-R. + #.076 RO2-N. + #.553 R2O2. + #.05 RCO-O2. + #.122 CO + #.024 CO2 + #.165 HCHO + #.001 CCHO + #.239 RCHO + #.273 MEK + #.283 PROD2 + #.156 HCOOH + #.967 XC
	7.06e-11	7.06e-11			PRD2 + HO. = #.216 HO2. + #.368 RO2-R. + #.123 RO2-N. + #.589 R2O2. + #.293 RCO-O2. + #.082 CO + #.017 HCHO + #.515 RCHO + #.165 MEK + #.2 PROD2 + #.006 HCOOH + #-2.264 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD2 + HV = #.415 HO2. + #1.425 RO2-R. + #.16 RO2-N. + #.034 R2O2. + CO + #.038 HCHO + #.001 RCHO + #.657 MEK + #.426 PROD2 + #.031 HCOOH + #-4.218 XC
3,6,9,12-Tetraoxahexadecan-1-ol [LP]	8.35e-11	8.35e-11			TETRAGBE + HO. = #.669 RO2-R. + #.331 RO2-N. + #.989 R2O2. + #.109 HCHO + #.005 CCHO + #.169 RCHO + #.369 MEK + #.913 PROD2 + #.008 HCOOH + #2.423 XC
3,6,9,12-Tetraoxahexadecan-1-ol [AP]	8.35e-11	8.35e-11			TETRAGBE + HO. = #.669 RO2-R. + #.331 RO2-N. + #.989 R2O2. + #.109 HCHO + #.005 CCHO + #.085 RCHO + #.369 MEK + #.008 HCOOH + #2.423 XC + #.913 PRD1 + #.084 PRD2
	3.17e-11	3.17e-11			PRD1 + HO. = #.156 HO2. + #.677 RO2-R. + #.135 RO2-N. + #.559 R2O2. + #.033 RCO-O2. + #.082 CO + #.016 CO2 + #.158 HCHO + #.006 CCHO + #.327 RCHO + #.421 MEK + #.369 PROD2 + #.103 HCOOH + #-0.291 XC
	7.78e-11	7.78e-11			PRD2 + HO. = #.207 HO2. + #.35 RO2-R. + #.169 RO2-N. + #.552 R2O2. + #.274 RCO-O2. + #.075 CO + #.012 HCHO + #.002 CCHO + #.557 RCHO + #.239 MEK + #.173 PROD2 + #.004 HCOOH + #-2.596 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.444 HO2. + #1.33 RO2-R. + #.226 RO2-N. + CO + #.035 HCHO + #.001 RCHO + #.606 MEK + #.376 PROD2 + #.029 HCOOH + #-4.102 XC
Methyl Formate	2.27e-13	2.27e-13			ME-FORM + HO. = RO2-R. + #.411 CO + #.071 CO2 + #.071 HCHO + #.411 HCOOH + #.518 INERT + #.518 XC
Ethyl Formate	1.02e-12	1.02e-12			ET-FORM + HO. = #.098 RO2-R. + #.902 R2O2. + #.748 CCO-O2. + #.154 RCO-O2. + #.061 CO2 + #.061 CCHO + #.014 RCHO + #.748 HCOOH + #.023 INERT + #.047 XC
Methyl Acetate	3.47e-13	8.30e-13	0.52		ME-ACET + HO. = #.985 RO2-R. + #.015 RO2-N. + #.368 CO + #.368 CCO-OH + #.617 INERT + #1.188 XC
Ethyl Acetate [LP]	1.60e-12	1.60e-12			ET-ACET + HO. = #.148 RO2-R. + #.04 RO2-N. + #.818 R2O2. + #.812 CCO-O2. + #.096 RCHO + #.018 MGLY + #.807 CCO-OH + #.005 RCO-OH + #.033 INERT + #.128 XC
Ethyl Acetate [AP]	1.60e-12	1.60e-12			ET-ACET + HO. = #.148 RO2-R. + #.04 RO2-N. + #.818 R2O2. + #.812 CCO-O2. + #.018 MGLY + #.807 CCO-OH + #.005 RCO-OH + #.033 INERT + #.128 XC + #.096 PRD1
	2.04e-11	2.04e-11			PRD1 + HO. = #.053 RO2-R. + #.002 RO2-N. + #.945 RCO-O2. + #.053 CO + #.047 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.985 RO2-R. + #.015 RO2-N. + #1.368 CO + #.368 CCO-OH + #.188 XC
Methyl Propionate [LP]	1.03e-12	1.03e-12			ME-PRAT + HO. = #.925 RO2-R. + #.043 RO2-N. + #.125 R2O2. + #.032 RCO-O2. + #.137 CO + #.032 CCHO + #.239 RCHO + #.042 MEK + #.02 PROD2 + #.326 BACL + #.117 RCO-OH + #.181 INERT + #.603 XC
Methyl Propionate [AP]	1.03e-12	1.03e-12			ME-PRAT + HO. = #.925 RO2-R. + #.043 RO2-N. + #.125 R2O2. + #.032 RCO-O2. + #.137 CO + #.032 CCHO + #.042 MEK + #.02 PROD2 + #.117 RCO-OH + #.181 INERT + #.603 XC + #.239 PRD1 + #.326 PRD2
	1.97e-11	1.97e-11			PRD1 + HO. = #.021 RO2-R. + #.001 RO2-N. + #.006 R2O2. + #.977 RCO-O2. + #.009 CO + #.015 RCHO + #.006 MGLY + #-0.012 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.786 HO2. + #1.214 RO2-R. + #1.066 CO + #.102 MEK + #.832 MGLY + #.066 RCO-OH + #-1.168 XC
	7.66e-13	7.66e-13			PRD2 + HO. = #.083 HO2. + #.719 RO2-R. + #.036 RO2-N. + #.161 R2O2. + #.162 RCO-O2. + #.236 CO + #.162 HCHO + #.121 MGLY + #.681 BACL + #-0.188 XC
		PF=BACL_ADJ			PRD2 + HV = CCO-O2. + RCO-O2. + #-1 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
n-Propyl Formate [LP]	2.38e-12	2.38e-12			C3-FORM + HO. = #.157 RO2-R. + #.039 RO2-N. + #.805 R2O2. + #.804 RCO-O2. + #.041 CO2 + #.001 HCHO + #.109 RCHO + #.033 MEK + #.367 HCOOH + #.014 INERT + #.468 XC
n-Propyl Formate [AP]	2.38e-12	2.38e-12			C3-FORM + HO. = #.157 RO2-R. + #.039 RO2-N. + #.805 R2O2. + #.804 RCO-O2. + #.041 CO2 + #.001 HCHO + #.041 RCHO + #.033 MEK + #.367 HCOOH + #.014 INERT + #.468 XC + #.068 PRD1
	2.11e-11	2.11e-11			PRD1 + HO. = #.036 RO2-R. + #.004 RO2-N. + #.051 R2O2. + #.961 RCO-O2. + #.029 CO + #.006 CO2 + #.036 RCHO + #.04 HCOOH + #-0.086 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.082 HO2. + RO2-R. + #.918 RCO-O2. + CO + #.082 RCHO + #-1 XC
Ethyl Propionate [LP]	2.14e-12	2.14e-12			ET-PRAT + HO. = #.199 RO2-R. + #.072 RO2-N. + #.839 R2O2. + #.727 CCO-O2. + #.002 RCO-O2. + #.002 CCHO + #.149 RCHO + #.028 MEK + #.094 PROD2 + #.022 BACL + #.633 RCO-OH + #-0.006 XC
Ethyl Propionate [AP]	2.14e-12	2.14e-12			ET-PRAT + HO. = #.199 RO2-R. + #.072 RO2-N. + #.839 R2O2. + #.727 CCO-O2. + #.002 RCO-O2. + #.002 CCHO + #.028 MEK + #.022 BACL + #.633 RCO-OH + #-0.006 XC + #.149 PRD1 + #.094 PRD2
	2.10e-11	2.10e-11			PRD1 + HO. = #.033 RO2-R. + #.006 RO2-N. + #.047 R2O2. + #.036 CCO-O2. + #.925 RCO-O2. + #.031 CO + #.038 RCHO + #.005 MEK + #.001 BACL + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.752 HO2. + #1.094 RO2-R. + #.045 RO2-N. + #.108 CCO-O2. + #1.181 CO + #.023 MEK + #.363 MGLY + #.289 RCO-OH + #-0.997 XC
	6.19e-12	6.19e-12			PRD2 + HO. = #.913 HO2. + #.087 RO2-R. + #.028 CO2 + #.035 HCHO + #.028 CCHO + #.051 RCHO + #.035 MGLY + #.885 BACL + #2.079 XC
Isopropyl Acetate [LP]	3.40e-12	3.40e-12			IPR-ACET + HO. = #.142 RO2-R. + #.075 RO2-N. + #.954 R2O2. + #.73 C-O2. + #.053 CCO-O2. + #.175 CO2 + #.058 HCHO + #.034 RCHO + #.175 ACET + #.106 MGLY + #.053 CCO-OH + #.557 INERT + #1.874 XC
Isopropyl Acetate [AP]	3.40e-12	3.40e-12			IPR-ACET + HO. = #.142 RO2-R. + #.075 RO2-N. + #.954 R2O2. + #.73 C-O2. + #.053 CCO-O2. + #.175 CO2 + #.058 HCHO + #.175 ACET + #.053 CCO-OH + #.557 INERT + #1.874 XC + #.034 PRD1 + #.106 PRD2
	2.18e-11	2.18e-11			PRD1 + HO. = #.101 RO2-R. + #.007 RO2-N. + #.892 RCO-O2. + #.101 CO + #.08 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.078 HO2. + #.96 RO2-R. + #.04 RO2-N. + #.922 CCO-O2. + CO + #.922 CCO-OH + #-1.965 XC
	5.41e-12	5.41e-12			PRD2 + HO. = #.002 HO2. + #.059 RO2-R. + #.004 RO2-N. + #.004 C-O2. + #.931 RCO-O2. + #.002 CO + #.002 CO2 + #.057 HCHO + #.002 ACET + #.063 MGLY + #-0.076 XC
		PF=MGLY_ADJ			PRD2 + HV = HO2. + RCO-O2. + CO + #-1 XC
Methyl Butyrate [LP]	3.04e-12	3.04e-12			ME-BUAT + HO. = #.918 RO2-R. + #.067 RO2-N. + #.171 R2O2. + #.015 RCO-O2. + #.054 CO + #.001 HCHO + #.096 CCHO + #.099 RCHO + #.558 MEK + #.007 PROD2 + #.08 MGLY + #.142 BACL + #.047 RCO-OH + #.785 XC
Methyl Butyrate [AP]	3.04e-12	3.04e-12			ME-BUAT + HO. = #.918 RO2-R. + #.067 RO2-N. + #.171 R2O2. + #.015 RCO-O2. + #.054 CO + #.001 HCHO + #.096 CCHO + #.015 RCHO + #.558 MEK + #.007 PROD2 + #.047 RCO-OH + #.785 XC + #.084 PRD1 + #.08 PRD2 + #.142 PRD3

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.07e-11	2.07e-11			PRD1 + HO. = #.063 RO2-R. + #.005 RO2-N. + #.005 R2O2. + #.933 RCO-O2. + #.043 CO + #.053 RCHO + #.013 BACL + #-0.079 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.961 RO2-R. + #.039 RO2-N. + CO + #.961 RCHO + #-1.118 XC
	5.11e-12	5.11e-12			PRD2 + HO. = #.041 RO2-R. + #.002 R2O2. + #.959 RCO-O2. + #.016 CO + #.041 MGLY + #-0.016 XC
		PF=MGLY_ADJ			PRD2 + HV = HO2. + RCO-O2. + CO + #-1 XC
	1.47e-12	1.47e-12			PRD3 + HO. = #.497 RO2-R. + #.065 RO2-N. + #.444 R2O2. + #.438 RCO-O2. + #.056 CO + #.009 HCHO + #.435 CCHO + #.002 MGLY + #.494 BACL + #-0.624 XC
		PF=BACL_ADJ			PRD3 + HV = #2 RCO-O2. + #-2 XC
Methyl Isobutyrate [LP]	1.73e-12	1.73e-12			ME-IBUAT + HO. = #.378 RO2-R. + #.075 RO2-N. + #.771 R2O2. + #.547 RCO-O2. + #.082 CO + #.106 HCHO + #.008 CCHO + #.081 RCHO + #.539 ACET + #.135 MEK + #.005 PROD2 + #.081 BACL + #.077 RCO-OH + #-0.276 XC
Methyl Isobutyrate [AP]	1.73e-12	1.73e-12			ME-IBUAT + HO. = #.378 RO2-R. + #.075 RO2-N. + #.771 R2O2. + #.547 RCO-O2. + #.082 CO + #.106 HCHO + #.008 CCHO + #.539 ACET + #.135 MEK + #.005 PROD2 + #.077 RCO-OH + #-0.276 XC + #.081 PRD1 + #.081 PRD2
	2.01e-11	2.01e-11			PRD1 + HO. = #.032 RO2-R. + #.002 RO2-N. + #.002 R2O2. + #.966 RCO-O2. + #.024 CO + #.012 RCHO + #.02 BACL + #-0.052 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.737 HO2. + #1.142 RO2-R. + #.047 RO2-N. + #.074 RCO-O2. + #1.046 CO + #.074 CCHO + #.071 MEK + #.046 PROD2 + #.761 BACL + #-2.307 XC
	3.26e-13	3.26e-13			PRD2 + HO. = #.784 RO2-R. + #.039 RO2-N. + #.176 R2O2. + #.176 RCO-O2. + #.257 CO + #.176 HCHO + #.131 MGLY + #.653 BACL + #-0.205 XC
		PF=BACL_ADJ			PRD2 + HV = CCO-O2. + RCO-O2. + #-1 XC
n-Butyl Formate [LP]	3.12e-12	3.12e-12			C4-FORM + HO. = #.334 RO2-R. + #.073 RO2-N. + #.831 R2O2. + #.593 RCO-O2. + #.014 CO2 + #.119 CCHO + #.063 RCHO + #.199 MEK + #.072 PROD2 + #.16 HCOOH + #.954 XC
n-Butyl Formate [AP]	3.12e-12	3.12e-12			C4-FORM + HO. = #.334 RO2-R. + #.073 RO2-N. + #.831 R2O2. + #.593 RCO-O2. + #.014 CO2 + #.119 CCHO + #.199 MEK + #.16 HCOOH + #.954 XC + #.063 PRD1 + #.072 PRD2
	2.91e-11	2.91e-11			PRD1 + HO. = #.243 HO2. + #.074 RO2-R. + #.005 RO2-N. + #.678 RCO-O2. + #.028 CO + #.317 RCHO + #-0.073 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.966 HO2. + #.98 RO2-R. + #.039 RO2-N. + #.014 RCO-O2. + CO + #.024 HCHO + #.942 RCHO + #-1.134 XC
	5.97e-12	5.97e-12			PRD2 + HO. = #.651 HO2. + #.279 RO2-R. + #.019 RO2-N. + #.051 RCO-O2. + #.223 HCHO + #.925 RCHO + #.006 BACL + #2.711 XC
Propyl Acetate [LP]	3.40e-12	3.40e-12			PR-ACET + HO. = #.433 RO2-R. + #.066 RO2-N. + #.552 R2O2. + #.501 RCO-O2. + #.007 CO + #.001 HCHO + #.038 CCHO + #.05 RCHO + #.344 MEK + #.002 MGLY + #.499 CCO-OH + #.01 RCO-OH + #.031 INERT + #.43 XC
Propyl Acetate [AP]	3.40e-12	3.40e-12			PR-ACET + HO. = #.433 RO2-R. + #.066 RO2-N. + #.552 R2O2. + #.501 RCO-O2. + #.007 CO + #.001 HCHO + #.038 CCHO + #.344 MEK + #.002 MGLY + #.499 CCO-OH + #.01 RCO-OH + #.031 INERT + #.43 XC + #.05 PRD1
	2.20e-11	2.20e-11			PRD1 + HO. = #.042 RO2-R. + #.008 RO2-N. + #.076 R2O2. + #.95 RCO-O2. + #.039 CO + #.002 HCHO + #.04 RCHO + #.074 CCO-OH + #-0.209 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 RCHO + #-1.12 XC
Ethyl Butyrate [LP]	4.94e-12	4.94e-12			ET-BUAT + HO. = #.424 RO2-R. + #.108 RO2-N. + #.616 R2O2. + #.466 CCO-O2. + #.002 RCO-O2. + #.001 HCHO + #.053 CCHO + #.093 RCHO + #.276 MEK + #.066 PROD2 + #.038 MGLY + #.019 BACL + #.4 RCO-OH + #1.14 XC
Ethyl Butyrate [AP]	4.94e-12	4.94e-12			ET-BUAT + HO. = #.424 RO2-R. + #.108 RO2-N. + #.616 R2O2. + #.466 CCO-O2. + #.002 RCO-O2. + #.001 HCHO + #.053 CCHO + #.002 RCHO + #.276 MEK + #.019 BACL + #.4 RCO-OH + #1.14 XC + #.092 PRD1 + #.038 PRD2 + #.066 PRD3
	2.21e-11	2.21e-11			PRD1 + HO. = #.075 RO2-R. + #.013 RO2-N. + #.053 R2O2. + #.034 CCO-O2. + #.878 RCO-O2. + #.05 CO + #.004 CCHO + #.073 RCHO + #.032 MEK + #.001 MGLY + #.003 BACL + #-0.202 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.974 HO2. + #.959 RO2-R. + #.067 RO2-N. + #1.175 CO + #.464 RCHO + #.293 MEK + #.001 BACL + #.175 RCO-OH + #-1.669 XC
	6.56e-12	6.56e-12			PRD2 + HO. = #.033 RO2-R. + #.01 RO2-N. + #.212 R2O2. + #.212 CCO-O2. + #.745 RCO-O2. + #.245 MGLY + #-0.454 XC
		PF=MGLY_ADJ			PRD2 + HV = HO2. + RCO-O2. + CO + #-1 XC
	1.06e-11	1.06e-11			PRD3 + HO. = #.641 HO2. + #.345 RO2-R. + #.014 RO2-N. + #.017 CO2 + #.326 CCHO + #.032 RCHO + #.326 MGLY + #.624 BACL + #.004 RCO-OH + #1.665 XC
Isobutyl Acetate	4.61e-12	4.61e-12			IBU-ACET + HO. = #.811 RO2-R. + #.12 RO2-N. + #.89 R2O2. + #.008 C-O2. + #.06 RCO-O2. + #.171 CO + #.052 HCHO + #.003 CCHO + #.015 RCHO + #.754 ACET + #.054 MEK + #.232 CCO-OH + #.591 INERT + #1.28 XC
Methyl Pivalate	1.27e-12	1.27e-12			ME-PVAT + HO. = #.365 RO2-R. + #.172 RO2-N. + #1.115 R2O2. + #.463 RCO-O2. + #.131 CO + #.576 HCHO + #.031 RCHO + #.463 ACET + #.203 MEK + #.131 RCO-OH + #.186 XC
n-Butyl Acetate [LP]	4.20e-12	4.20e-12			BU-ACET + HO. = #.675 RO2-R. + #.12 RO2-N. + #.516 R2O2. + #.205 RCO-O2. + #.006 CO + #.116 CCHO + #.172 RCHO + #.252 MEK + #.251 PROD2 + #.211 CCO-OH + #.024 INERT + #.95 XC
n-Butyl Acetate [AP]	4.20e-12	4.20e-12			BU-ACET + HO. = #.675 RO2-R. + #.12 RO2-N. + #.516 R2O2. + #.205 RCO-O2. + #.006 CO + #.116 CCHO + #.03 RCHO + #.252 MEK + #.211 CCO-OH + #.024 INERT + #.95 XC + #.142 PRD1 + #.251 PRD2
	2.35e-11	2.35e-11			PRD1 + HO. = #.081 HO2. + #.055 RO2-R. + #.003 RO2-N. + #.862 RCO-O2. + #.047 CO + #.093 RCHO + #.02 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.996 HO2. + #.978 RO2-R. + #.026 RO2-N. + #1.29 CO + #.007 HCHO + #.195 RCHO + #.29 CCO-OH + #-0.107 XC
	6.44e-12	6.44e-12			PRD2 + HO. = #.33 HO2. + #.14 RO2-R. + #.065 RO2-N. + #.508 R2O2. + #.106 CCO-O2. + #.36 RCO-O2. + #.154 HCHO + #.497 RCHO + #.024 BACL + #.351 CCO-OH + #1.821 XC
		PF=KETONE QY = 1.1e-2			PRD2 + HV = #.96 RO2-R. + #.04 RO2-N. + CCO-O2. + #.96 RCHO + #.88 XC
n-Propyl Propionate [LP]	4.02e-12	4.02e-12			PR-PRAT + HO. = #.421 RO2-R. + #.105 RO2-N. + #.574 R2O2. + #.474 RCO-O2. + #.006 CO + #.001 HCHO + #.034 CCHO + #.085 RCHO + #.296 MEK + #.051 PROD2 + #.011 BACL + #.428 RCO-OH + #.024 INERT + #.78 XC
n-Propyl Propionate [AP]	4.02e-12	4.02e-12			PR-PRAT + HO. = #.421 RO2-R. + #.105 RO2-N. + #.574 R2O2. + #.474 RCO-O2. + #.006 CO + #.001 HCHO + #.034 CCHO + #.296 MEK + #.011 BACL + #.428 RCO-OH + #.024 INERT + #.78 XC + #.085 PRD1 + #.051 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.25e-11	2.25e-11			PRD1 + HO. = #.047 RO2-R. + #.014 RO2-N. + #.083 R2O2. + #.939 RCO-O2. + #.019 CO + #.001 HCHO + #.003 CCHO + #.08 RCHO + #.004 PROD2 + #.001 BACL + #.035 RCO-OH + #-0.302 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.497 HO2. + #1.056 RO2-R. + #.092 RO2-N. + #.289 R2O2. + #.355 RCO-O2. + CO + #.013 CCHO + #.465 RCHO + #.03 MEK + #.058 MGLY + #.355 RCO-OH + #-2.397 XC
	6.19e-12	6.19e-12			PRD2 + HO. = #.913 HO2. + #.087 RO2-R. + #.028 CO2 + #.035 HCHO + #.028 CCHO + #.051 RCHO + #.035 MGLY + #.885 BACL + #2.079 XC
s-Butyl Acetate	5.50e-12	5.50e-12			SBU-ACET + HO. = #.714 RO2-R. + #.11 RO2-N. + #1.06 R2O2. + #.171 CCO-O2. + #.005 RCO-O2. + #.006 HCHO + #.834 CCHO + #.048 RCHO + #.011 MEK + #.176 CCO-OH + #.655 INERT + #2.115 XC
t-Butyl Acetate [LP]	4.25e-13	4.25e-13			TBU-ACET + HO. = #.156 RO2-R. + #.179 RO2-N. + #1.57 R2O2. + #.666 C-O2. + #.159 CO2 + #.811 HCHO + #.159 ACET + #.156 MGLY + #.506 INERT + #1.84 XC
t-Butyl Acetate [AP]	4.25e-13	4.25e-13			TBU-ACET + HO. = #.156 RO2-R. + #.179 RO2-N. + #1.57 R2O2. + #.666 C-O2. + #.159 CO2 + #.811 HCHO + #.159 ACET + #.506 INERT + #1.84 XC + #.156 PRD1
	5.40e-12	5.40e-12			PRD1 + HO. = #.001 HO2. + #.035 RO2-R. + #.009 RO2-N. + #.072 R2O2. + #.007 C-O2. + #.948 RCO-O2. + #.003 CO + #.003 CO2 + #.069 HCHO + #.003 ACET + #.04 MGLY + #-0.108 XC
		PF=MGLY_ADJ			PRD1 + HV = HO2. + RCO-O2. + CO + #-1 XC
Butyl Propionate [LP]	5.06e-12	5.06e-12			BU-PRAT + HO. = #.624 RO2-R. + #.168 RO2-N. + #.533 R2O2. + #.208 RCO-O2. + #.005 CO + #.102 CCHO + #.177 RCHO + #.222 MEK + #.243 PROD2 + #.006 BACL + #.19 RCO-OH + #.02 INERT + #1.666 XC
Butyl Propionate [AP]	5.06e-12	5.06e-12			BU-PRAT + HO. = #.624 RO2-R. + #.168 RO2-N. + #.533 R2O2. + #.208 RCO-O2. + #.005 CO + #.102 CCHO + #.027 RCHO + #.222 MEK + #.006 BACL + #.19 RCO-OH + #.02 INERT + #1.666 XC + #.15 PRD1 + #.243 PRD2
	2.39e-11	2.39e-11			PRD1 + HO. = #.063 HO2. + #.073 RO2-R. + #.011 RO2-N. + #.025 R2O2. + #.853 RCO-O2. + #.043 CO + #.004 CCHO + #.105 RCHO + #.006 MEK + #.002 BACL + #-0.058 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.777 HO2. + #1.059 RO2-R. + #.082 RO2-N. + #.099 R2O2. + #.082 RCO-O2. + #1.231 CO + #.005 HCHO + #.153 RCHO + #.033 MEK + #.044 PROD2 + #.02 MGLY + #.001 BACL + #.313 RCO-OH + #-1.193 XC
	6.88e-12	6.88e-12			PRD2 + HO. = #.29 HO2. + #.159 RO2-R. + #.098 RO2-N. + #.509 R2O2. + #.097 CCO-O2. + #.356 RCO-O2. + #.134 HCHO + #.002 CCHO + #.46 RCHO + #.012 MEK + #.014 PROD2 + #.037 BACL + #.331 RCO-OH + #1.319 XC
		PF=KETONE QY = 5.5e-3			PRD2 + HV = #.935 RO2-R. + #.065 RO2-N. + CCO-O2. + #.935 RCHO + #.805 XC
Amyl Acetate [LP]	6.05e-12	6.05e-12			AM-ACET + HO. = #.762 RO2-R. + #.222 RO2-N. + #.741 R2O2. + #.016 RCO-O2. + #.019 CCHO + #.214 RCHO + #.637 PROD2 + #.016 CCO-OH + #1.088 XC
Amyl Acetate [AP]	6.05e-12	6.05e-12			AM-ACET + HO. = #.762 RO2-R. + #.222 RO2-N. + #.741 R2O2. + #.016 RCO-O2. + #.019 CCHO + #.089 RCHO + #.016 CCO-OH + #1.088 XC + #.125 PRD1 + #.637 PRD2
	2.04e-11	2.04e-11			PRD1 + HO. = #.053 RO2-R. + #.002 RO2-N. + #.945 RCO-O2. + #.053 CO + #.047 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = HO2. + #.985 RO2-R. + #.015 RO2-N. + #1.368 CO + #.368 CCO-OH + #.188 XC
	1.21e-11	1.21e-11			PRD2 + HO. = #.484 HO2. + #.272 RO2-R. + #.062 RO2-N. + #.133 R2O2. + #.011 CCO-O2. + #.17 RCO-O2. + #.104 HCHO + #.057 CCHO + #.341 RCHO + #.454 MEK + #.002 PROD2 + #.005 BACL + #.098 CCO-OH + #1.738 XC
		PF=KETONE QY = 1.6e-3			PRD2 + HV = #.96 RO2-R. + #.04 RO2-N. + RCO-O2. + #.96 RCHO + #-0.12 XC
n-Propyl Butyrate [LP]	7.41e-12	7.41e-12			PR-BUAT + HO. = #.482 RO2-R. + #.148 RO2-N. + #.517 R2O2. + #.37 RCO-O2. + #.004 CO + #.001 HCHO + #.06 CCHO + #.062 RCHO + #.403 MEK + #.042 PROD2 + #.004 MGLY + #.011 BACL + #.332 RCO-OH + #1.784 XC
n-Propyl Butyrate [AP]	7.41e-12	7.41e-12			PR-BUAT + HO. = #.482 RO2-R. + #.148 RO2-N. + #.517 R2O2. + #.37 RCO-O2. + #.004 CO + #.001 HCHO + #.06 CCHO + #.001 RCHO + #.403 MEK + #.004 MGLY + #.011 BACL + #.332 RCO-OH + #1.784 XC + #.061 PRD1 + #.042 PRD2
	2.36e-11	2.36e-11			PRD1 + HO. = #.079 RO2-R. + #.026 RO2-N. + #.096 R2O2. + #.895 RCO-O2. + #.033 CO + #.001 HCHO + #.006 CCHO + #.111 RCHO + #.001 MEK + #.005 PROD2 + #.002 BACL + #.035 RCO-OH + #-0.368 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.902 RO2-R. + #.098 RO2-N. + CO + #.902 RCHO + #-1.293 XC
	1.06e-11	1.06e-11			PRD2 + HO. = #.641 HO2. + #.345 RO2-R. + #.014 RO2-N. + #.017 CO2 + #.326 CCHO + #.032 RCHO + #.326 MGLY + #.624 BACL + #.004 RCO-OH + #1.665 XC
2,3-Dimethyl-butyl Acetate	7.71e-12	7.71e-12			23MC4ACT + HO. = #.747 RO2-R. + #.247 RO2-N. + #1.02 R2O2. + #.006 RCO-O2. + #.005 CO + #.018 HCHO + #.183 CCHO + #.037 RCHO + #.716 ACET + #.549 MEK + #.006 PROD2 + #.011 CCO-OH + #.203 INERT + #1.4 XC
2-Methylpentyl Acetate	7.73e-12	7.73e-12			2MC5-ACT + HO. = #.703 RO2-R. + #.289 RO2-N. + #.906 R2O2. + #.008 RCO-O2. + #.009 CO + #.002 HCHO + #.012 CCHO + #.436 RCHO + #.212 MEK + #.252 PROD2 + #.017 CCO-OH + #.095 INERT + #2.413 XC
3-Methylpentyl Acetate	7.73e-12	7.73e-12			3MC5-ACT + HO. = #.73 RO2-R. + #.258 RO2-N. + #.877 R2O2. + #.011 RCO-O2. + #.001 HCHO + #.179 CCHO + #.386 RCHO + #.31 MEK + #.352 PROD2 + #.011 CCO-OH + #.001 INERT + #1.517 XC
4-Methylpentyl Acetate	7.45e-12	7.45e-12			4MC5-ACT + HO. = #.5 RO2-R. + #.293 RO2-N. + #1.029 R2O2. + #.207 RCO-O2. + #.005 HCHO + #.197 RCHO + #.145 ACET + #.175 MEK + #.139 PROD2 + #.207 CCO-OH + #.009 INERT + #2.632 XC
Isobutyl Isobutyrate	5.52e-12	5.52e-12			IBU-IBTR + HO. = #.68 RO2-R. + #.235 RO2-N. + #.927 R2O2. + #.006 C-O2. + #.079 RCO-O2. + #.12 CO + #.069 HCHO + #.002 CCHO + #.034 RCHO + #.649 ACET + #.542 MEK + #.003 PROD2 + #.003 BACL + #.18 RCO-OH + #1.366 XC
n-Butyl Butyrate [LP]	1.06e-11	1.06e-11			BU-BUAT + HO. = #.613 RO2-R. + #.214 RO2-N. + #.487 R2O2. + #.173 RCO-O2. + #.004 CO + #.104 CCHO + #.135 RCHO + #.313 MEK + #.194 PROD2 + #.003 MGLY + #.007 BACL + #.157 RCO-OH + #2.661 XC
n-Butyl Butyrate [AP]	1.06e-11	1.06e-11			BU-BUAT + HO. = #.613 RO2-R. + #.214 RO2-N. + #.487 R2O2. + #.173 RCO-O2. + #.004 CO + #.104 CCHO + #.022 RCHO + #.313 MEK + #.003 MGLY + #.007 BACL + #.157 RCO-OH + #2.661 XC + #.112 PRD1 + #.194 PRD2
	2.20e-11	2.20e-11			PRD1 + HO. = #.107 RO2-R. + #.014 RO2-N. + #.026 R2O2. + #.879 RCO-O2. + #.063 CO + #.008 CCHO + #.04 RCHO + #.063 MEK + #.001 MGLY + #.003 BACL + #-0.187 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.949 HO2. + #.983 RO2-R. + #.068 RO2-N. + #1.348 CO + #.583 MEK + #.001 BACL + #.348 RCO-OH + #-2.136 XC
	8.11e-12	8.11e-12			PRD2 + HO. = #.228 HO2. + #.245 RO2-R. + #.138 RO2-N. + #.46 R2O2. + #.082 CCO-O2. + #.306 RCO-O2. + #.108 HCHO + #.02 CCHO + #.376 RCHO + #.044 MEK + #.112 PROD2 + #.009 MGLY + #.032 BACL + #.284 RCO-OH + #.96 XC
n-Hexyl Acetate	7.47e-12	7.47e-12			NC6-ACET + HO. = #.682 RO2-R. + #.309 RO2-N. + #.805 R2O2. + #.009 RCO-O2. + #.058 RCHO + #.646 PROD2 + #.009 CCO-OH + #2.054 XC
Ethyl 3-Ethoxy Propionate [LP]	1.96e-11	1.96e-11			E3EOC3OH + HO. = #.404 RO2-R. + #.159 RO2-N. + #.987 R2O2. + #.278 C-O2. + #.159 CCO-O2. + #.002 HCHO + #.058 CCHO + #.056 RCHO + #.729 MEK + #.079 PROD2 + #.315 MGLY + #.001 BACL + #.093 RCO-OH + #.553 XC
Ethyl 3-Ethoxy Propionate [AP]	1.96e-11	1.96e-11			E3EOC3OH + HO. = #.404 RO2-R. + #.159 RO2-N. + #.987 R2O2. + #.278 C-O2. + #.159 CCO-O2. + #.002 HCHO + #.058 CCHO + #.729 MEK + #.001 BACL + #.093 RCO-OH + #.553 XC + #.056 PRD1 + #.315 PRD2 + #.079 PRD3
	2.11e-11	2.11e-11			PRD1 + HO. = #.003 RO2-R. + #.006 RO2-N. + #.082 R2O2. + #.073 CCO-O2. + #.918 RCO-O2. + #.076 RCHO + #.001 MGLY + #-0.164 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.544 HO2. + #1.191 RO2-R. + #.049 RO2-N. + #.216 CCO-O2. + CO + #.008 MEK + #.726 MGLY + #.216 RCO-OH + #-1.589 XC
	6.56e-12	6.56e-12			PRD2 + HO. = #.033 RO2-R. + #.01 RO2-N. + #.212 R2O2. + #.212 CCO-O2. + #.745 RCO-O2. + #.245 MGLY + #-0.454 XC
		PF=MGLY_ADJ			PRD2 + HV = HO2. + RCO-O2. + CO + #-1 XC
	3.91e-11	3.91e-11			PRD3 + HO. = #.78 RO2-R. + #.066 RO2-N. + #.904 R2O2. + #.154 C-O2. + #.001 HCHO + #.032 CCHO + #.031 RCHO + #.726 MEK + #.03 PROD2 + #.727 MGLY + #.004 BACL + #.142 RCO-OH + #-0.417 XC
2,4-Dimethyl-pentyl Acetate	9.13e-12	9.13e-12			24MC5ACT + HO. = #.584 RO2-R. + #.397 RO2-N. + #1.289 R2O2. + #.019 RCO-O2. + #.005 CO + #.152 HCHO + #.019 CCHO + #.267 RCHO + #.048 ACET + #.247 MEK + #.191 PROD2 + #.024 CCO-OH + #.247 INERT + #2.991 XC
2-Methylhexyl Acetate	9.15e-12	9.15e-12			2MC6-ACT + HO. = #.63 RO2-R. + #.364 RO2-N. + #.922 R2O2. + #.005 RCO-O2. + #.002 CO + #.001 HCHO + #.045 CCHO + #.143 RCHO + #.107 MEK + #.495 PROD2 + #.008 CCO-OH + #.084 INERT + #2.777 XC
3-Ethylpentyl Acetate	9.56e-12	9.56e-12			3EC5-ACT + HO. = #.686 RO2-R. + #.309 RO2-N. + #.852 R2O2. + #.005 RCO-O2. + #.001 HCHO + #.173 CCHO + #.338 RCHO + #.232 MEK + #.397 PROD2 + #.005 CCO-OH + #.001 INERT + #2.449 XC
3-Methylhexyl Acetate	9.15e-12	9.15e-12			3MC6-ACT + HO. = #.655 RO2-R. + #.338 RO2-N. + #.819 R2O2. + #.007 RCO-O2. + #.001 HCHO + #.01 CCHO + #.301 RCHO + #.112 MEK + #.445 PROD2 + #.007 CCO-OH + #.001 INERT + #2.892 XC
4-Methylhexyl Acetate	9.15e-12	9.15e-12			4MC6-ACT + HO. = #.453 RO2-R. + #.359 RO2-N. + #1.057 R2O2. + #.189 RCO-O2. + #.001 HCHO + #.11 CCHO + #.133 RCHO + #.195 MEK + #.195 PROD2 + #.189 CCO-OH + #.009 INERT + #3.328 XC
5-Methylhexyl Acetate	8.87e-12	8.87e-12			5MC6-ACT + HO. = #.628 RO2-R. + #.365 RO2-N. + #.821 R2O2. + #.007 RCO-O2. + #.003 CO + #.008 HCHO + #.089 RCHO + #.013 ACET + #.565 PROD2 + #.01 CCO-OH + #.005 INERT + #3.055 XC
Isoamyl Isobutyrate [LP]	6.94e-12	6.94e-12			IC5IBUAT + HO. = #.58 RO2-R. + #.294 RO2-N. + #.843 R2O2. + #.125 RCO-O2. + #.028 HCHO + #.455 RCHO + #.434 ACET + #.032 MEK + #.113 PROD2 + #.002 BACL + #.109 RCO-OH + #3.018 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Isoamyl Isobutyrate [AP]	6.94e-12	6.94e-12			IC5IBUAT + HO. = #.58 RO2-R. + #.294 RO2-N. + #.843 R2O2. + #.125 RCO-O2. + #.028 HCHO + #.434 ACET + #.032 MEK + #.002 BACL + #.109 RCO-OH + #3.018 XC + #.455 PRD1 + #.113 PRD2
	2.24e-11	2.24e-11			PRD1 + HO. = #.026 HO2. + #.079 RO2-R. + #.013 RO2-N. + #.037 R2O2. + #.883 RCO-O2. + #.068 CO + #.008 HCHO + #.035 RCHO + #.007 ACET + #.067 MEK + #.003 PROD2 + #.001 BACL + #-0.218 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.898 HO2. + #1.02 RO2-R. + #.079 RO2-N. + #.002 RCO-O2. + #1.315 CO + #.022 HCHO + #.032 CCHO + #.007 RCHO + #.002 ACET + #.569 MEK + #.027 PROD2 + #.315 RCO-OH + #-2.297 XC
	8.60e-12	8.60e-12			PRD2 + HO. = #.359 HO2. + #.468 RO2-R. + #.115 RO2-N. + #.058 RCO-O2. + #.35 HCHO + #.023 CCHO + #.499 RCHO + #.056 ACET + #.281 MEK + #.021 MGLY + #.026 BACL + #1.781 XC
n-Heptyl Acetate	8.89e-12	8.89e-12			NC7-ACET + HO. = #.623 RO2-R. + #.369 RO2-N. + #.797 R2O2. + #.007 RCO-O2. + #.009 RCHO + #.614 PROD2 + #.007 CCO-OH + #3.035 XC
2,4-Dimethyl-hexyl Acetate	1.08e-11	1.08e-11			24MC6ACT + HO. = #.504 RO2-R. + #.479 RO2-N. + #1.386 R2O2. + #.017 RCO-O2. + #.002 CO + #.012 HCHO + #.285 CCHO + #.132 RCHO + #.173 MEK + #.295 PROD2 + #.019 CCO-OH + #.27 INERT + #3.33 XC
2-Ethyl-Hexyl Acetate [LP]	1.10e-11	1.10e-11			2ETHXACT + HO. = #.581 RO2-R. + #.415 RO2-N. + #.933 R2O2. + #.004 RCO-O2. + #.002 CO + #.096 CCHO + #.127 RCHO + #.075 MEK + #.476 PROD2 + #.006 CCO-OH + #.064 INERT + #3.692 XC
2-Ethyl-Hexyl Acetate [AP]	1.10e-11	1.10e-11			2ETHXACT + HO. = #.581 RO2-R. + #.415 RO2-N. + #.933 R2O2. + #.004 RCO-O2. + #.002 CO + #.096 CCHO + #.005 RCHO + #.075 MEK + #.006 CCO-OH + #.064 INERT + #3.692 XC + #.122 PRD1 + #.476 PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	1.39e-11	1.39e-11			PRD2 + HO. = #.211 HO2. + #.547 RO2-R. + #.17 RO2-N. + #.054 R2O2. + #.048 CCO-O2. + #.025 RCO-O2. + #.006 HCHO + #.118 CCHO + #.376 RCHO + #.253 MEK + #.429 PROD2 + #.001 CCO-OH + #-0.282 XC
		PF=KETONE QY = 7.2e-4			PRD2 + HV = #.93 RO2-R. + #.07 RO2-N. + #.785 R2O2. + RCO-O2. + #.93 RCHO + #-0.211 XC
3,4-Dimethylhexyl Acetate	1.08e-11	1.08e-11			34MC6ACT + HO. = #.592 RO2-R. + #.373 RO2-N. + #1.064 R2O2. + #.034 RCO-O2. + #.008 HCHO + #.308 CCHO + #.109 RCHO + #.274 MEK + #.508 PROD2 + #.034 CCO-OH + #.01 INERT + #2.483 XC
3,5-Dimethylhexyl Acetate	1.06e-11	1.06e-11			35MC6ACT + HO. = #.576 RO2-R. + #.419 RO2-N. + #1.103 R2O2. + #.006 RCO-O2. + #.097 HCHO + #.014 CCHO + #.337 RCHO + #.041 ACET + #.008 MEK + #.483 PROD2 + #.006 CCO-OH + #3.263 XC
3-Ethylhexyl Acetate	1.10e-11	1.10e-11			3EC6-ACT + HO. = #.623 RO2-R. + #.374 RO2-N. + #.82 R2O2. + #.003 RCO-O2. + #.001 HCHO + #.043 CCHO + #.276 RCHO + #.546 PROD2 + #.003 CCO-OH + #.001 INERT + #3.551 XC
3-Methylheptyl Aceate	1.06e-11	1.06e-11			3MC7-ACT + HO. = #.582 RO2-R. + #.412 RO2-N. + #.843 R2O2. + #.006 RCO-O2. + #.001 HCHO + #.034 CCHO + #.079 RCHO + #.56 PROD2 + #.006 CCO-OH + #3.835 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b]				Reactions and Products [c]
	k(298)	A	Ea	B	
4,5-Dimethylhexyl Acetate	1.06e-11	1.06e-11			45MC6ACT + HO. = #.522 RO2-R. + #.397 RO2-N. + #1.117 R2O2. + #.081 RCO-O2. + #.005 HCHO + #.087 CCHO + #.134 RCHO + #.323 ACET + #.101 MEK + #.312 PROD2 + #.081 CCO-OH + #.012 INERT + #3.373 XC
4-Methylheptyl Acetate	1.06e-11	1.06e-11			4MC7-ACT + HO. = #.441 RO2-R. + #.408 RO2-N. + #.984 R2O2. + #.15 RCO-O2. + #.001 HCHO + #.001 CCHO + #.086 RCHO + #.112 MEK + #.308 PROD2 + #.15 CCO-OH + #.008 INERT + #4.235 XC
5-Methylheptyl Aceate	1.06e-11	1.06e-11			5MC7-ACT + HO. = #.585 RO2-R. + #.409 RO2-N. + #.836 R2O2. + #.006 RCO-O2. + #.003 CO + #.001 HCHO + #.044 CCHO + #.058 RCHO + #.012 MEK + #.543 PROD2 + #.009 CCO-OH + #.005 INERT + #3.934 XC
n-Octyl Acetate	1.03e-11	1.03e-11			NC8-ACET + HO. = #.585 RO2-R. + #.409 RO2-N. + #.784 R2O2. + #.006 RCO-O2. + #.008 RCHO + #.577 PROD2 + #.006 CCO-OH + #4.031 XC
2,3,5-Teimethyl-hexyl Acetate	1.22e-11	1.22e-11			235M6ACT + HO. = #.541 RO2-R. + #.457 RO2-N. + #1.288 R2O2. + #.002 RCO-O2. + #.004 CO + #.04 HCHO + #.063 CCHO + #.058 RCHO + #.063 ACET + #.376 MEK + #.484 PROD2 + #.006 CCO-OH + #.134 INERT + #3.168 XC
2,3-Dimethyl-heptyl Acetate	1.23e-11	1.23e-11			23MC7ACT + HO. = #.569 RO2-R. + #.429 RO2-N. + #1.065 R2O2. + #.002 RCO-O2. + #.004 CO + #.002 HCHO + #.068 CCHO + #.071 RCHO + #.289 MEK + #.527 PROD2 + #.006 CCO-OH + #.092 INERT + #3.638 XC
2,4-Dimethyl-heptyl Acetate	1.23e-11	1.23e-11			24MC7ACT + HO. = #.479 RO2-R. + #.507 RO2-N. + #1.28 R2O2. + #.015 RCO-O2. + #.001 CO + #.008 HCHO + #.003 CCHO + #.302 RCHO + #.045 MEK + #.41 PROD2 + #.015 CCO-OH + #.227 INERT + #4.099 XC
2,5-Dimethyl-heptyl Acetate	1.23e-11	1.23e-11			25MC7ACT + HO. = #.533 RO2-R. + #.463 RO2-N. + #1.235 R2O2. + #.004 RCO-O2. + #.018 CO + #.003 HCHO + #.162 CCHO + #.089 RCHO + #.217 MEK + #.45 PROD2 + #.022 CCO-OH + #.121 INERT + #3.868 XC
2-Methyloctyl Acetate	1.20e-11	1.20e-11			2MC8-ACT + HO. = #.538 RO2-R. + #.458 RO2-N. + #.931 R2O2. + #.004 RCO-O2. + #.001 CO + #.002 CCHO + #.077 RCHO + #.041 MEK + #.476 PROD2 + #.005 CCO-OH + #.043 INERT + #4.931 XC
3,5-Dimethyl-heptyl Acetate	1.23e-11	1.23e-11			35MC7ACT + HO. = #.491 RO2-R. + #.504 RO2-N. + #1.242 R2O2. + #.005 RCO-O2. + #.005 HCHO + #.227 CCHO + #.266 RCHO + #.012 MEK + #.451 PROD2 + #.005 CCO-OH + #3.942 XC
3,6-Dimethyl-heptyl Acetate	1.20e-11	1.20e-11			36MC7ACT + HO. = #.519 RO2-R. + #.476 RO2-N. + #1.16 R2O2. + #.005 RCO-O2. + #.012 HCHO + #.006 CCHO + #.251 RCHO + #.148 ACET + #.493 PROD2 + #.005 CCO-OH + #3.935 XC
3-Ethylheptyl Acetate	1.24e-11	1.24e-11			3EC7-ACT + HO. = #.556 RO2-R. + #.442 RO2-N. + #.849 R2O2. + #.003 RCO-O2. + #.049 CCHO + #.074 RCHO + #.536 PROD2 + #.003 CCO-OH + #4.8 XC
4,5-Dimethyl-heptyl Acetate	1.23e-11	1.23e-11			45MC7ACT + HO. = #.521 RO2-R. + #.431 RO2-N. + #1.136 R2O2. + #.048 RCO-O2. + #.003 HCHO + #.21 CCHO + #.08 RCHO + #.235 MEK + #.471 PROD2 + #.048 CCO-OH + #.01 INERT + #3.738 XC
4,6-Dimethylheptyl Acetate	1.20e-11	1.20e-11			46MC7ACT + HO. = #.423 RO2-R. + #.452 RO2-N. + #1.123 R2O2. + #.125 RCO-O2. + #.037 HCHO + #.009 CCHO + #.178 RCHO + #.022 ACET + #.007 MEK + #.372 PROD2 + #.125 CCO-OH + #.006 INERT + #4.744 XC
4-Methyloctyl Acetate	1.20e-11	1.20e-11			4MC8-ACT + HO. = #.469 RO2-R. + #.438 RO2-N. + #.919 R2O2. + #.093 RCO-O2. + #.01 CCHO + #.064 RCHO + #.453 PROD2 + #.093 CCO-OH + #.005 INERT + #4.97 XC
5-Methyloctyl Acetate	1.20e-11	1.20e-11			5MC8-ACT + HO. = #.558 RO2-R. + #.436 RO2-N. + #.831 R2O2. + #.005 RCO-O2. + #.002 CO + #.001 CCHO + #.087 RCHO + #.003 MEK + #.53 PROD2 + #.007 CCO-OH + #.004 INERT + #4.888 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b]				Reactions and Products [c]
	k(298)	A	Ea	B	
n-Nonyl Acetate	1.17e-11	1.17e-11			NC9-ACET + HO. = #.56 RO2-R. + #.435 RO2-N. + #.777 R2O2. + #.005 RCO-O2. + #.007 RCHO + #.553 PROD2 + #.005 CCO-OH + #5.026 XC
3,6-Dimethyl-octyl Acetate	1.37e-11	1.37e-11			36MC8ACT + HO. = #.522 RO2-R. + #.474 RO2-N. + #1.101 R2O2. + #.004 RCO-O2. + #.002 HCHO + #.107 CCHO + #.187 RCHO + #.071 MEK + #.514 PROD2 + #.004 CCO-OH + #4.988 XC
3-Isopropyl-heptyl Acetate	1.38e-11	1.38e-11			3IPC7ACT + HO. = #.548 RO2-R. + #.449 RO2-N. + #.958 R2O2. + #.003 RCO-O2. + #.001 HCHO + #.012 CCHO + #.117 RCHO + #.247 ACET + #.502 PROD2 + #.003 CCO-OH + #5.161 XC
4,6-Dimethyl-octyl Acetate	1.37e-11	1.37e-11			46MC8ACT + HO. = #.428 RO2-R. + #.494 RO2-N. + #1.158 R2O2. + #.078 RCO-O2. + #.003 HCHO + #.136 CCHO + #.194 RCHO + #.013 MEK + #.393 PROD2 + #.078 CCO-OH + #.004 INERT + #5.374 XC
3,5,7-Trimethyl-octyl Acetate	1.51e-11	1.51e-11			357M8ACT + HO. = #.462 RO2-R. + #.534 RO2-N. + #1.185 R2O2. + #.004 RCO-O2. + #.008 HCHO + #.006 CCHO + #.368 RCHO + #.041 ACET + #.001 MEK + #.394 PROD2 + #.004 CCO-OH + #6.168 XC
3-Ethyl-6-Methyloctyl Acetate	1.55e-11	1.55e-11			3E6M8ACT + HO. = #.507 RO2-R. + #.491 RO2-N. + #1.092 R2O2. + #.002 RCO-O2. + #.001 HCHO + #.137 CCHO + #.139 RCHO + #.072 MEK + #.5 PROD2 + #.002 CCO-OH + #6.061 XC
4,7-Dimethyl-nonyl Acetate	1.51e-11	1.51e-11			47MC9ACT + HO. = #.382 RO2-R. + #.502 RO2-N. + #1.12 R2O2. + #.116 RCO-O2. + #.001 HCHO + #.055 CCHO + #.083 RCHO + #.044 MEK + #.352 PROD2 + #.116 CCO-OH + #.006 INERT + #6.761 XC
2,3,5,7-Tetramethyloctyl Acetate	1.68e-11	1.68e-11			2357M8AC + HO. = #.466 RO2-R. + #.533 RO2-N. + #1.267 R2O2. + #.001 RCO-O2. + #.003 CO + #.021 HCHO + #.047 CCHO + #.166 RCHO + #.016 ACET + #.281 MEK + #.426 PROD2 + #.005 CCO-OH + #.078 INERT + #6.371 XC
3,5,7-Trimethylnonyl Acetate	1.68e-11	1.68e-11			357M9ACT + HO. = #.451 RO2-R. + #.545 RO2-N. + #1.181 R2O2. + #.003 RCO-O2. + #.002 HCHO + #.089 CCHO + #.285 RCHO + #.03 MEK + #.383 PROD2 + #.003 CCO-OH + #7.258 XC
3,6,8-Trimethylnonyl Acetate	1.65e-11	1.65e-11			368M9ACT + HO. = #.477 RO2-R. + #.52 RO2-N. + #1.132 R2O2. + #.004 RCO-O2. + #.039 HCHO + #.005 CCHO + #.218 RCHO + #.022 ACET + #.001 MEK + #.463 PROD2 + #.004 CCO-OH + #7.313 XC
2,4,6,8-Tetramethylnonyl Acetate	1.82e-11	1.82e-11			2468M8AC + HO. = #.44 RO2-R. + #.553 RO2-N. + #1.208 R2O2. + #.007 RCO-O2. + #.001 CO + #.008 HCHO + #.005 CCHO + #.25 RCHO + #.02 ACET + #.068 MEK + #.34 PROD2 + #.008 CCO-OH + #.072 INERT + #8.431 XC
3-Ethyl-6,7-Dimethylnonyl Acetate	1.86e-11	1.86e-11			3E67M9AC + HO. = #.501 RO2-R. + #.497 RO2-N. + #1.13 R2O2. + #.002 RCO-O2. + #.191 CCHO + #.077 RCHO + #.197 MEK + #.504 PROD2 + #.002 CCO-OH + #7.581 XC
4,7,9-Trimethyldecyl Acetate	1.79e-11	1.79e-11			479M10AC + HO. = #.374 RO2-R. + #.53 RO2-N. + #1.149 R2O2. + #.096 RCO-O2. + #.025 HCHO + #.001 CCHO + #.106 RCHO + #.016 ACET + #.001 MEK + #.351 PROD2 + #.096 CCO-OH + #.005 INERT + #8.831 XC
2,3,5,6,8-Pentaamethylnonyl Acetate	1.99e-11	1.99e-11			23568M9A + HO. = #.447 RO2-R. + #.552 RO2-N. + #1.36 R2O2. + #.001 RCO-O2. + #.003 CO + #.017 HCHO + #.037 CCHO + #.076 RCHO + #.028 ACET + #.233 MEK + #.65 PROD2 + #.004 CCO-OH + #.05 INERT + #7.386 XC
3,5,7,9-Tetramethyldecyl Acetate	1.96e-11	1.96e-11			3579M10A + HO. = #.439 RO2-R. + #.558 RO2-N. + #1.149 R2O2. + #.003 RCO-O2. + #.006 HCHO + #.005 CCHO + #.22 RCHO + #.021 ACET + #.406 PROD2 + #.003 CCO-OH + #9.461 XC
5-Ethyl-3,6,8-Trimethylnonyl Acetate	2.00e-11	2.00e-11			5E368M9A + HO. = #.427 RO2-R. + #.57 RO2-N. + #1.315 R2O2. + #.003 RCO-O2. + #.018 HCHO + #.062 CCHO + #.146 RCHO + #.024 ACET + #.008 MEK + #.671 PROD2 + #.003 CCO-OH + #7.854 XC
Dimethyl Carbonate	3.30e-13	3.30e-13			DMC + HO. = RO2-R. + #.393 CO + #.393 RCO-OH + #.607 INERT + #.82 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Propylene Carbonate [LP]	6.90e-13	6.90e-13			PC + HO. = #.627 RO2-R. + #.021 RO2-N. + #1.511 R2O2. + #.353 CCO-O2. + #.225 CO + #.213 HCHO + #.034 RCHO + #.577 RCO-OH + #.368 INERT + #.53 XC
Propylene Carbonate [AP]	6.90e-13	6.90e-13			PC + HO. = #.627 RO2-R. + #.021 RO2-N. + #1.511 R2O2. + #.353 CCO-O2. + #.225 CO + #.213 HCHO + #.577 RCO-OH + #.368 INERT + #.53 XC + #.034 PRD1
	2.22e-11	2.22e-11			PRD1 + HO. = #.128 RO2-R. + #.007 RO2-N. + #.051 R2O2. + #.865 RCO-O2. + #.128 CO + #.106 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.038 HO2. + #1.962 RO2-R. + #1.378 CO + #.378 RCO-OH + #-0.135 XC
Methyl Lactate [LP]	2.76e-12	2.76e-12			ME-LACT + HO. = #.835 HO2. + #.153 RO2-R. + #.006 RO2-N. + #.005 RCO-O2. + #.023 CO + #.061 HCHO + #.005 CCHO + #.036 MEK + #.023 PROD2 + #.061 MGLY + #.868 BACL + #-0.088 XC
Methyl Lactate [AP]	2.76e-12	2.76e-12			ME-LACT + HO. = #.835 HO2. + #.153 RO2-R. + #.006 RO2-N. + #.005 RCO-O2. + #.023 CO + #.061 HCHO + #.005 CCHO + #.036 MEK + #.023 PROD2 + #-0.088 XC + #.061 PRD1 + #.868 PRD2
	5.11e-12	5.11e-12			PRD1 + HO. = #.041 RO2-R. + #.002 R2O2. + #.959 RCO-O2. + #.016 CO + #.041 MGLY + #-0.016 XC
		PF=MGLY_ADJ			PRD1 + HV = HO2. + RCO-O2. + CO + #-1 XC
	5.20e-13	5.20e-13			PRD2 + HO. = #.036 HO2. + #.755 RO2-R. + #.038 RO2-N. + #.17 R2O2. + #.17 RCO-O2. + #.248 CO + #.17 HCHO + #.127 MGLY + #.665 BACL + #-0.197 XC
		PF=BACL_ADJ			PRD2 + HV = CCO-O2. + RCO-O2. + #-1 XC
2-Methoxyethyl Acetate [LP]	1.26e-11	1.26e-11			MCSVACET + HO. = #.818 RO2-R. + #.077 RO2-N. + #.854 R2O2. + #.105 RCO-O2. + #.262 CO + #.005 HCHO + #.003 RCHO + #.079 MEK + #.02 PROD2 + #.368 CCO-OH + #1.179 INERT + #1.596 XC
2-Methoxyethyl Acetate [AP]	1.26e-11	1.26e-11			MCSVACET + HO. = #.818 RO2-R. + #.077 RO2-N. + #.854 R2O2. + #.105 RCO-O2. + #.262 CO + #.005 HCHO + #.003 RCHO + #.079 MEK + #.02 PROD2 + #.368 CCO-OH + #1.179 INERT + #1.596 XC
Ethyl Lactate [LP]	3.91e-12	3.91e-12			ET-LACT + HO. = #.175 HO2. + #.452 RO2-R. + #.031 RO2-N. + #.342 CCO-O2. + #.001 RCO-O2. + #.039 HCHO + #.001 CCHO + #.039 RCHO + #.013 MEK + #.342 PROD2 + #.039 MGLY + #.536 BACL + #-0.391 XC
Ethyl Lactate [AP]	3.91e-12	3.91e-12			ET-LACT + HO. = #.175 HO2. + #.452 RO2-R. + #.031 RO2-N. + #.342 CCO-O2. + #.001 RCO-O2. + #.039 HCHO + #.001 CCHO + #.013 MEK + #-0.391 XC + #.039 PRD1 + #.536 PRD2 + #.342 PRD3 + #.039 PRD4
	6.56e-12	6.56e-12			PRD1 + HO. = #.033 RO2-R. + #.01 RO2-N. + #.212 R2O2. + #.212 CCO-O2. + #.745 RCO-O2. + #.245 MGLY + #-0.454 XC
		PF=MGLY_ADJ			PRD1 + HV = HO2. + RCO-O2. + CO + #-1 XC
	1.78e-12	1.78e-12			PRD2 + HO. = #.142 RO2-R. + #.065 RO2-N. + #.793 R2O2. + #.761 CCO-O2. + #.032 RCO-O2. + #.032 HCHO + #.023 MGLY + #.88 BACL + #-1.629 XC
		PF=BACL_ADJ			PRD2 + HV = CCO-O2. + RCO-O2. + #-1 XC
	6.19e-12	6.19e-12			PRD3 + HO. = #.913 HO2. + #.087 RO2-R. + #.028 CO2 + #.035 HCHO + #.028 CCHO + #.051 RCHO + #.035 MGLY + #.885 BACL + #2.079 XC
	2.28e-11	2.28e-11			PRD4 + HO. = #.094 HO2. + #.047 RO2-R. + #.003 RO2-N. + #.856 RCO-O2. + #.047 CO + #.047 MEK + #.094 BACL + #-0.197 XC
	3.80e-15	3.80e-15			PRD4 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD4 + HV = HO2. + #.961 RO2-R. + #.039 RO2-N. + #1.244 CO + #.376 MEK + #.244 PROD2 + #.34 BACL + #-2.812 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Methyl Isopropyl Carbonate	2.55e-12	2.55e-12			MIPR-CB + HO. = #.302 RO2-R. + #.047 RO2-N. + #.707 R2O2. + #.599 C-O2. + #.052 CCO-O2. + #.023 CO + #.209 CO2 + #.265 HCHO + #.033 RCHO + #.209 ACET + #.035 MEK + #.075 RCO-OH + #.601 INERT + #1.825 XC
1-Methoxy-2-Propyl Acetate [LP]	1.44e-11	1.44e-11			PGME-ACT + HO. = #.324 RO2-R. + #.127 RO2-N. + #1.4 R2O2. + #.542 CCO-O2. + #.006 RCO-O2. + #.031 HCHO + #.003 RCHO + #.049 MEK + #.05 PROD2 + #.549 CCO-OH + INERT + #1.499 XC
1-Methoxy-2-Propyl Acetate [AP]	1.44e-11	1.44e-11			PGME-ACT + HO. = #.324 RO2-R. + #.127 RO2-N. + #1.4 R2O2. + #.542 CCO-O2. + #.006 RCO-O2. + #.031 HCHO + #.003 RCHO + #.049 MEK + #.549 CCO-OH + INERT + #1.499 XC + #.05 PRD1
	5.06e-12	5.06e-12			PRD1 + HO. = #.051 RO2-R. + #.099 RO2-N. + #.902 R2O2. + #.016 CCO-O2. + #.834 RCO-O2. + #.007 CO + #.012 CO2 + #.018 HCHO + #.025 RCHO + #.007 MEK + #.159 HCOOH + #.02 CCO-OH + #2.485 XC
2-Ethoxyethyl Acetate [LP]	1.94e-11	1.94e-11			CSV-ACET + HO. = #.573 RO2-R. + #.112 RO2-N. + #.843 R2O2. + #.29 C-O2. + #.026 RCO-O2. + #.166 CO + #.004 HCHO + #.059 CCHO + #.055 RCHO + #.746 MEK + #.064 PROD2 + #.192 CCO-OH + #.284 INERT + #.473 XC
2-Ethoxyethyl Acetate [AP]	1.94e-11	1.94e-11			CSV-ACET + HO. = #.573 RO2-R. + #.112 RO2-N. + #.843 R2O2. + #.29 C-O2. + #.026 RCO-O2. + #.166 CO + #.004 HCHO + #.059 CCHO + #.746 MEK + #.064 PROD2 + #.192 CCO-OH + #.284 INERT + #.473 XC + #.055 PRD1
	2.04e-11	2.04e-11			PRD1 + HO. = #.053 RO2-R. + #.002 RO2-N. + #.945 RCO-O2. + #.053 CO + #.047 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.985 RO2-R. + #.015 RO2-N. + #1.368 CO + #.368 CCO-OH + #.188 XC
2-Methyoxy-1-propyl Acetate	2.30e-11	2.30e-11			2PGMEACT + HO. = #.827 RO2-R. + #.11 RO2-N. + #.93 R2O2. + #.06 C-O2. + #.003 RCO-O2. + #.289 CO + #.011 HCHO + #.011 CCHO + #.043 MEK + #.001 PROD2 + #.001 HCOOH + #.291 CCO-OH + #1.404 INERT + #2.785 XC
Dimethyl Succinate [LP]	1.50e-12	1.50e-12			DBE-4 + HO. = #.899 RO2-R. + #.085 RO2-N. + #.07 R2O2. + #.016 RCO-O2. + #.31 CO + #.016 RCHO + #.516 MEK + #.002 PROD2 + #.073 BACL + #.308 RCO-OH + #1.792 XC
Dimethyl Succinate [AP]	1.50e-12	1.50e-12			DBE-4 + HO. = #.899 RO2-R. + #.085 RO2-N. + #.07 R2O2. + #.016 RCO-O2. + #.31 CO + #.016 RCHO + #.516 MEK + #.002 PROD2 + #.308 RCO-OH + #1.792 XC + #.073 PRD1
	6.65e-13	6.65e-13			PRD1 + HO. = #.874 RO2-R. + #.118 RO2-N. + #.214 R2O2. + #.008 RCO-O2. + #.286 CO + #.008 MGLY + #.874 BACL + #-0.538 XC
		PF=BACL_ADJ			PRD1 + HV = #2 RCO-O2. + #-2 XC
Ethylene Glycol Diacetate [LP]	3.78e-12	3.78e-12			ETGLDACT + HO. = #.094 RO2-R. + #.1 RO2-N. + #.842 R2O2. + #.806 RCO-O2. + #.006 CO + #.074 MEK + #.003 MGLY + #.798 CCO-OH + #.014 RCO-OH + #.028 INERT + #1.005 XC
Ethylene Glycol Diacetate [AP]	3.78e-12	3.78e-12			ETGLDACT + HO. = #.094 RO2-R. + #.1 RO2-N. + #.842 R2O2. + #.806 RCO-O2. + #.006 CO + #.074 MEK + #.003 MGLY + #.798 CCO-OH + #.014 RCO-OH + #.028 INERT + #1.005 XC
Diisopropyl Carbonate [LP]	6.88e-12	6.88e-12			DIPR-CB + HO. = #.251 RO2-R. + #.139 RO2-N. + #.647 R2O2. + #.577 C-O2. + #.033 CCO-O2. + #.202 CO2 + #.038 HCHO + #.048 RCHO + #.403 ACET + #.579 MEK + #.033 RCO-OH + #1.519 XC
Diisopropyl Carbonate [AP]	6.88e-12	6.88e-12			DIPR-CB + HO. = #.251 RO2-R. + #.139 RO2-N. + #.647 R2O2. + #.577 C-O2. + #.033 CCO-O2. + #.202 CO2 + #.038 HCHO + #.403 ACET + #.579 MEK + #.033 RCO-OH + #1.519 XC + #.048 PRD1
	2.52e-11	2.52e-11			PRD1 + HO. = #.113 RO2-R. + #.032 RO2-N. + #.093 R2O2. + #.079 C-O2. + #.006 CCO-O2. + #.769 RCO-O2. + #.108 CO + #.028 CO2 + #.007 HCHO + #.028 CCHO + #.091 RCHO + #.028 ACET + #.081 MEK + #-0.468 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.131 HO2. + #.902 RO2-R. + #.098 RO2-N. + #.869 CCO-O2. + CO + #.033 MEK + #.869 RCO-OH + #-3.064 XC
Dimethyl Glutarate [LP]	3.50e-12	3.50e-12			DBE-5 + HO. = #.827 RO2-R. + #.173 RO2-N. + #.172 R2O2. + #.153 CO + #.601 MEK + #.153 PROD2 + #.073 BACL + #2.194 XC
Dimethyl Glutarate [AP]	3.50e-12	3.50e-12			DBE-5 + HO. = #.827 RO2-R. + #.173 RO2-N. + #.172 R2O2. + #.153 CO + #.601 MEK + #2.194 XC + #.153 PRD1 + #.073 PRD2
	7.14e-12	7.14e-12			PRD1 + HO. = #.108 HO2. + #.801 RO2-R. + #.087 RO2-N. + #.404 R2O2. + #.003 RCO-O2. + #.025 CO + #.026 CO2 + #.448 RCHO + #.018 MEK + #.035 PROD2 + #.39 MGLY + #.242 BACL + #.2 RCO-OH + #1.054 XC
	7.61e-12	7.61e-12			PRD2 + HO. = #.57 HO2. + #.269 RO2-R. + #.042 RO2-N. + #.119 RCO-O2. + #.017 CO + #.097 RCHO + #.861 BACL + #-0.362 XC
		PF=BACL_ADJ			PRD2 + HV = #2 RCO-O2. + #-2 XC
2-Butoxyethyl Acetate [LP]	2.38e-11	2.38e-11			2BUETACT + HO. = #.779 RO2-R. + #.206 RO2-N. + #.899 R2O2. + #.016 RCO-O2. + #.142 CO + #.017 CCHO + #.369 RCHO + #.674 MEK + #.116 PROD2 + #.157 CCO-OH + #.239 INERT + #1.488 XC
2-Butoxyethyl Acetate [AP]	2.38e-11	2.38e-11			2BUETACT + HO. = #.779 RO2-R. + #.206 RO2-N. + #.899 R2O2. + #.016 RCO-O2. + #.142 CO + #.017 CCHO + #.369 RCHO + #.674 MEK + #.157 CCO-OH + #.239 INERT + #1.488 XC + #.116 PRD1
	1.36e-11	1.36e-11			PRD1 + HO. = #.838 HO2. + #.126 RO2-R. + #.009 RO2-N. + #.027 RCO-O2. + #.001 CO2 + #.042 CCHO + #.086 RCHO + #.395 MEK + #.015 HCOOH + #.002 CCO-OH + #3.386 XC
Dimethyl Adipate [LP]	8.80e-12	8.80e-12			DBE-6 + HO. = #.782 RO2-R. + #.218 RO2-N. + #.623 R2O2. + #.036 CO + #.879 RCHO + #.181 MEK + #.035 PROD2 + #.02 MGLY + #.126 BACL + #.002 RCO-OH + #2.519 XC
Dimethyl Adipate [AP]	8.80e-12	8.80e-12			DBE-6 + HO. = #.782 RO2-R. + #.218 RO2-N. + #.623 R2O2. + #.036 CO + #.181 MEK + #.02 MGLY + #.002 RCO-OH + #2.519 XC + #.035 PRD1 + #.126 PRD2 + #.879 PRD3
	7.44e-12	7.44e-12			PRD1 + HO. = #.83 RO2-R. + #.17 RO2-N. + #.696 R2O2. + #.01 CO + #.014 CO2 + #1.044 RCHO + #.001 MEK + #.06 PROD2 + #.027 MGLY + #.124 BACL + #.112 RCO-OH + #.546 XC
	8.54e-12	8.54e-12			PRD2 + HO. = #.237 HO2. + #.563 RO2-R. + #.118 RO2-N. + #.082 RCO-O2. + #.014 CO + #.081 RCHO + #.432 MGLY + #.801 BACL + #-1.713 XC
		PF=BACL_ADJ			PRD2 + HV = #2 RCO-O2. + #-2 XC
	1.97e-11	1.97e-11			PRD3 + HO. = #.021 RO2-R. + #.001 RO2-N. + #.006 R2O2. + #.977 RCO-O2. + #.009 CO + #.015 RCHO + #.006 MGLY + #-0.012 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.786 HO2. + #1.214 RO2-R. + #1.066 CO + #.102 MEK + #.832 MGLY + #.066 RCO-OH + #-1.168 XC
2-(2-Ethoxy-ethoxy) ethyl acetate [LP]	3.86e-11	3.86e-11			DGEEA + HO. = #.698 RO2-R. + #.211 RO2-N. + #.947 R2O2. + #.079 C-O2. + #.011 RCO-O2. + #.079 CO + #.021 HCHO + #.027 CCHO + #.009 RCHO + #.846 MEK + #.406 PROD2 + #.002 HCOOH + #.091 CCO-OH + #.134 INERT + #.298 XC
2-(2-Ethoxy-ethoxy) ethyl acetate [AP]	3.86e-11	3.86e-11			DGEEA + HO. = #.698 RO2-R. + #.211 RO2-N. + #.947 R2O2. + #.079 C-O2. + #.011 RCO-O2. + #.079 CO + #.021 HCHO + #.027 CCHO + #.009 RCHO + #.846 MEK + #.002 HCOOH + #.091 CCO-OH + #.134 INERT + #.298 XC + #.406 PRD1
	1.71e-11	1.71e-11			PRD1 + HO. = #.241 HO2. + #.459 RO2-R. + #.067 RO2-N. + #.677 R2O2. + #.167 C-O2. + #.003 CCO-O2. + #.063 RCO-O2. + #.168 CO + #.026 CO2 + #.025 HCHO + #.035 CCHO + #.004 RCHO + #.578 MEK + #.033 PROD2 + #.158 HCOOH + #.034 CCO-OH + #1.717 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
2-(2-Butoxy-ethoxy) ethyl acetate [LP]	4.29e-11	4.29e-11			DGBEA + HO. = #.711 RO2-R. + #.279 RO2-N. + #.863 R2O2. + #.01 RCO-O2. + #.062 CO + #.014 HCHO + #.009 CCHO + #.185 RCHO + #.649 MEK + #.443 PROD2 + #.072 CCO-OH + #.106 INERT + #2.143 XC
2-(2-Butoxy-ethoxy) ethyl acetate [AP]	4.29e-11	4.29e-11			DGBEA + HO. = #.711 RO2-R. + #.279 RO2-N. + #.863 R2O2. + #.01 RCO-O2. + #.062 CO + #.014 HCHO + #.009 CCHO + #.185 RCHO + #.649 MEK + #.072 CCO-OH + #.106 INERT + #2.143 XC + #.443 PRD1
	2.09e-11	2.09e-11			PRD1 + HO. = #.157 HO2. + #.688 RO2-R. + #.126 RO2-N. + #.755 R2O2. + #.029 RCO-O2. + #.198 CO + #.025 CO2 + #.024 HCHO + #.015 CCHO + #.169 RCHO + #.666 MEK + #.072 PROD2 + #.15 HCOOH + #.068 CCO-OH + #.609 XC
1-Hydroxy-2,2,4-Trimethyl-pentyl-3-Isobutyrate [LP]	1.29e-11	1.29e-11			TEXANOL2 + HO. = #.754 RO2-R. + #.242 RO2-N. + #.177 R2O2. + #.003 RCO-O2. + #.362 HCHO + #.001 CCHO + #.437 RCHO + #.361 ACET + #.345 MEK + #.009 PROD2 + #.001 RCO-OH + #6.342 XC
1-Hydroxy-2,2,4-Trimethyl-pentyl-3-Isobutyrate [AP]	1.29e-11	1.29e-11			TEXANOL2 + HO. = #.754 RO2-R. + #.242 RO2-N. + #.177 R2O2. + #.003 RCO-O2. + #.362 HCHO + #.001 CCHO + #.361 ACET + #.345 MEK + #.009 PROD2 + #.001 RCO-OH + #6.342 XC + #.437 PRD1
	2.74e-11	2.74e-11			PRD1 + HO. = #.188 RO2-R. + #.101 RO2-N. + #.239 R2O2. + #.711 RCO-O2. + #.137 CO + #.021 HCHO + #.003 CCHO + #.05 RCHO + #.22 ACET + #.14 MEK + #.003 PROD2 + #.001 MGLY + #-1.297 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.059 HO2. + #1.465 RO2-R. + #.392 RO2-N. + #.287 R2O2. + #.084 RCO-O2. + CO + #1.279 ACET + #.54 MEK + #.084 RCO-OH + #-6.85 XC
3-Hydroxy-2,2,4-Trimethy-lpentyl-1-Isobutyrate [LP]	1.62e-11	1.62e-11			TEXANOL1 + HO. = #.439 HO2. + #.43 RO2-R. + #.126 RO2-N. + #.004 RCO-O2. + #.003 CO + #.034 HCHO + #.01 CCHO + #.244 RCHO + #.218 ACET + #.12 MEK + #.628 PROD2 + #.001 BACL + #.003 RCO-OH + #5.532 XC
3-Hydroxy-2,2,4-Trimethyl-pentyl-1-Isobutyrate [AP]	1.62e-11	1.62e-11			TEXANOL1 + HO. = #.439 HO2. + #.43 RO2-R. + #.126 RO2-N. + #.004 RCO-O2. + #.003 CO + #.034 HCHO + #.01 CCHO + #.218 ACET + #.12 MEK + #.001 BACL + #.003 RCO-OH + #5.532 XC + #.244 PRD1 + #.628 PRD2
	2.41e-11	2.41e-11			PRD1 + HO. = #.089 RO2-R. + #.023 RO2-N. + #.073 R2O2. + #.888 RCO-O2. + #.084 CO + #.015 HCHO + #.005 CCHO + #.005 RCHO + #.076 ACET + #.049 MEK + #-0.348 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #.539 HO2. + #1.314 RO2-R. + #.138 RO2-N. + #.007 C-O2. + #.001 RCO-O2. + #1.143 CO + #.884 ACET + #.256 MEK + #.143 RCO-OH + #-3.09 XC
	1.04e-11	1.04e-11			PRD2 + HO. = #.032 RO2-R. + #.366 RO2-N. + #1.259 R2O2. + #.602 RCO-O2. + #.148 HCHO + #.043 CCHO + #.031 RCHO + #.501 ACET + #.515 MEK + #-1.895 XC
Ethylene Oxide	7.60e-14	7.60e-14			ETOX + HO. = RO2-R. + R2O2. + #.411 CO + #.071 CO2 + #.071 HCHO + #.411 HCOOH + #.518 INERT + #.518 XC
Propylene Oxide	5.20e-13	5.20e-13			PROX + HO. = #.765 RO2-R. + #.008 RO2-N. + #1.441 R2O2. + #.227 CCO-O2. + #.282 CO + #.034 CO2 + #.235 HCHO + #.018 CCHO + #.006 RCHO + #.317 HCOOH + #.192 CCO-OH + #.443 INERT + #.748 XC
1,2-Epoxy-butane	1.91e-12	1.91e-12			12BUOX + HO. = #.797 RO2-R. + #.059 RO2-N. + #1.746 R2O2. + #.144 RCO-O2. + #.312 CO + #.054 CO2 + #.039 HCHO + #.554 CCHO + #.014 RCHO + #.011 MEK + #.371 HCOOH + #.084 RCO-OH + #.42 INERT + #.568 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Formic Acid	4.50e-13	4.50e-13			FORMACID + HO. = HO2. + CO2
Acetic Acid [LP]	8.00e-13	8.00e-13			ACETACID + HO. = #.491 RO2-R. + #.509 C-O2. + #.509 CO2 + #.491 MGLY + #-0.491 XC
Acetic Acid [AP]	8.00e-13	8.00e-13			ACETACID + HO. = #.491 RO2-R. + #.509 C-O2. + #.509 CO2 + #-0.491 XC + #.491 PRD1
	1.17e-11	1.17e-11			PRD1 + HO. = RCO-O2.
		PF=MGLY_ADJ			PRD1 + HV = #2 HO2. + CO + CO2 + XC
Acrylic Acid [LP]	2.84e-11	2.84e-11			ACYRACID + HO. = RO2-R. + #.015 CO2 + #.548 HCHO + #.015 CCHO + #.208 RCHO + #.548 MGLY + #.229 BACL + #-0.777 XC
	1.01e-17	1.01e-17			ACYRACID + O3 = #.11 HO. + #.11 HO2. + #.3 CO + #.115 CO2 + #.5 HCHO + #.5 MGLY + #.185 HCOOH + #.45 INERT + #-0.05 XC
	2.76e-18	2.76e-18			ACYRACID + NO3 = RO2-R. + #.062 CO2 + #.062 RCHO + #.938 BACL + #-1 XC + XN
	4.60e-12	4.60e-12			ACYRACID + O3P = #.45 RCHO + #.55 RCO-OH + #-0 XC
Acrylic Acid [AP]	2.84e-11	2.84e-11			ACYRACID + HO. = RO2-R. + #.015 CO2 + #.548 HCHO + #.015 CCHO + #-0.777 XC + #.229 PRD1 + #.548 PRD2 + #.208 PRD3
	1.01e-17	1.01e-17			ACYRACID + O3 = #.11 HO. + #.11 HO2. + #.3 CO + #.115 CO2 + #.5 HCHO + #.185 HCOOH + #.45 INERT + #-0.05 XC + #.5 PRD2
	2.76e-18	2.76e-18			ACYRACID + NO3 = RO2-R. + #.062 CO2 + #-1 XC + #.938 PRD4 + #.062 PRD5 + XN
	4.60e-12	4.60e-12			ACYRACID + O3P = #.55 RCO-OH + #-0 XC + #.45 PRD6
	3.11e-12	3.11e-12			PRD1 + HO. = #.864 HO2. + #.136 RCO-O2. + #.034 CO2 + #.101 HCHO + #.864 MGLY + #.864 XC
		PF=BACL_ADJ			PRD1 + HV = HO2. + RCO-O2. + CO2
	1.17e-11	1.17e-11			PRD2 + HO. = RCO-O2.
		PF=MGLY_ADJ			PRD2 + HV = #2 HO2. + CO + CO2 + XC
	6.49e-11	6.49e-11			PRD3 + HO. = #.058 HO2. + #.942 RCO-O2. + #.058 MGLY
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #2 HO2. + CO + MGLY + #-1 XC
	1.36e-13	1.36e-13			PRD4 + HO. = #.213 NO2 + #.787 RCO-O2. + #.787 CO2 + #.213 MGLY + #.213 XC + #.787 XN
		PF=BACL_ADJ			PRD4 + HV = HO2. + RCO-O2. + CO2 + XN
	1.93e-11	1.93e-11			PRD5 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD5 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD5 + HV = NO2 + HO2. + CO + HCHO + XC
	6.11e-11	6.11e-11			PRD6 + HO. = RCO-O2.
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = HO2. + RO2-R. + CO + MGLY + #-1 XC
Propionic Acid [LP]	1.16e-12	1.16e-12			PROPACID + HO. = RO2-R. + #.142 CO2 + #.142 CCHO + #.4 RCHO + #.457 BACL + #-0.457 XC
Propionic Acid [AP]	1.16e-12	1.16e-12			PROPACID + HO. = RO2-R. + #.142 CO2 + #.142 CCHO + #-0.457 XC + #.4 PRD1 + #.457 PRD2
	6.11e-11	6.11e-11			PRD1 + HO. = RCO-O2.
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + RO2-R. + CO + MGLY + #-1 XC
	2.11e-13	2.11e-13			PRD2 + HO. = #.211 RO2-R. + #.283 R2O2. + #.506 CCO-O2. + #.283 RCO-O2. + #.506 CO2 + #.283 HCHO + #.211 MGLY + #.717 XC
		PF=BACL_ADJ			PRD2 + HV = HO2. + CCO-O2. + CO2 + XC
Methyl Acrylate [LP]	2.84e-11	2.84e-11			ME-ACRYL + HO. = #.948 RO2-R. + #.042 RO2-N. + #.085 R2O2. + #.01 RCO-O2. + #.016 CO + #.681 HCHO + #.01 CCHO + #.041 PROD2 + #.681 MGLY + #.225 BACL + #-0.194 XC
	1.01e-17	1.01e-17			ME-ACRYL + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 MGLY + #.185 HCOOH + #1.5 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	2.76e-18	2.76e-18			ME-ACRYL + NO3 = #.916 RO2-R. + #.05 RO2-N. + #.292 R2O2. + #.034 RCO-O2. + #.056 CO + #.034 RCHO + #.774 BACL + #.142 RNO3 + #-0.507 XC + #.858 XN
	4.60e-12	4.60e-12			ME-ACRYL + O3P = #.45 RCHO + #.55 MEK + #.45 XC
Methyl Acrylate [AP]	2.84e-11	2.84e-11			ME-ACRYL + HO. = #.948 RO2-R. + #.042 RO2-N. + #.085 R2O2. + #.01 RCO-O2. + #.016 CO + #.681 HCHO + #.01 CCHO + #-0.194 XC + #.225 PRD1 + #.681 PRD2 + #.041 PRD3
	1.01e-17	1.01e-17			ME-ACRYL + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #1.5 XC + #.5 PRD2
	2.76e-18	2.76e-18			ME-ACRYL + NO3 = #.916 RO2-R. + #.05 RO2-N. + #.292 R2O2. + #.034 RCO-O2. + #.056 CO + #.142 RNO3 + #-0.507 XC + #.774 PRD4 + #.034 PRD5 + #.858 XN
	4.60e-12	4.60e-12			ME-ACRYL + O3P = #.55 MEK + #.45 XC + #.45 PRD6
	3.93e-12	3.93e-12			PRD1 + HO. = #.851 HO2. + #.057 RO2-R. + #.002 RO2-N. + #.09 RCO-O2. + #.024 CO + #.09 HCHO + #.763 MGLY + #.145 BACL + #.735 XC
		PF=BACL_ADJ			PRD1 + HV = #2 RCO-O2. + #-2 XC
	5.11e-12	5.11e-12			PRD2 + HO. = #.041 RO2-R. + #.002 R2O2. + #.959 RCO-O2. + #.016 CO + #.041 MGLY + #-0.016 XC
		PF=MGLY_ADJ			PRD2 + HV = HO2. + RCO-O2. + CO + #-1 XC
	6.95e-12	6.95e-12			PRD3 + HO. = #.979 HO2. + #.021 RCO-O2. + #.028 HCHO + #.578 RCHO + #.028 MGLY + #.374 BACL + #2.598 XC
	9.54e-13	9.54e-13			PRD4 + HO. = #.1 NO2 + #.136 HO2. + #.734 RO2-R. + #.03 RO2-N. + #.291 CO + #.1 MGLY + #.87 BACL + #-0.251 XC + #.9 XN
		PF=BACL_ADJ			PRD4 + HV = #2 RCO-O2. + #-2 XC + XN
	1.93e-11	1.93e-11			PRD5 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD5 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD5 + HV = NO2 + HO2. + CO + HCHO + XC
	1.97e-11	1.97e-11			PRD6 + HO. = #.021 RO2-R. + #.001 RO2-N. + #.006 R2O2. + #.977 RCO-O2. + #.009 CO + #.015 RCHO + #.006 MGLY + #-0.012 XC
	3.80e-15	3.80e-15			PRD6 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD6 + HV = #.786 HO2. + #1.214 RO2-R. + #1.066 CO + #.102 MEK + #.832 MGLY + #.066 RCO-OH + #-1.168 XC
Vinyl Acetate [LP]	3.16e-11	3.16e-11			VIN-ACET + HO. = #.953 RO2-R. + #.039 RO2-N. + #.007 R2O2. + #.007 RCO-O2. + #.874 HCHO + #.079 RCHO + #.007 CCO-OH + #.874 INERT + #1.74 XC
	1.01e-17	1.01e-17			VIN-ACET + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #.5 INERT + #2.5 XC
	1.38e-14	1.38e-14			VIN-ACET + NO3 = #.08 RO2-R. + #.039 RO2-N. + #.88 R2O2. + #.88 RCO-O2. + #.88 CCO-OH + #-0.637 XC + XN
	5.60e-12	5.60e-12			VIN-ACET + O3P = #.45 RCHO + #.55 MEK + #.45 XC
Vinyl Acetate [AP]	3.16e-11	3.16e-11			VIN-ACET + HO. = #.953 RO2-R. + #.039 RO2-N. + #.007 R2O2. + #.007 RCO-O2. + #.874 HCHO + #.007 CCO-OH + #.874 INERT + #1.74 XC + #.079 PRD1
	1.01e-17	1.01e-17			VIN-ACET + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #.5 INERT + #2.5 XC
	1.38e-14	1.38e-14			VIN-ACET + NO3 = #.08 RO2-R. + #.039 RO2-N. + #.88 R2O2. + #.88 RCO-O2. + #.88 CCO-OH + #-0.637 XC + XN
	5.60e-12	5.60e-12			VIN-ACET + O3P = #.55 MEK + #.45 XC + #.45 PRD2
	2.75e-11	2.75e-11			PRD1 + HO. = #.296 HO2. + #.704 RCO-O2. + #.296 MGLY
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + XC
	2.04e-11	2.04e-11			PRD2 + HO. = #.053 RO2-R. + #.002 RO2-N. + #.945 RCO-O2. + #.053 CO + #.047 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD2 + HV = HO2. + #.985 RO2-R. + #.015 RO2-N. + #1.368 CO + #.368 CCO-OH + #.188 XC
2-Methyl-2-Butene-3-ol [LP]	6.35e-11	8.20e-12	-1.21		MBUTENOL + HO. = #.935 RO2-R. + #.065 RO2-N. + #.311 HCHO + #.624 CCHO + #.311 RCHO + #.624 ACET + #.246 XC
	9.30e-18	9.30e-18			MBUTENOL + O3 = #.099 HO. + #.099 HO2. + #.365 CO + #.091 CO2 + #.3 HCHO + #.7 RCHO + #.015 ACET + #.259 HCOOH + #.285 RCO-OH + #.985 XC
	1.20e-14	4.60e-14	0.80		MBUTENOL + NO3 = #.935 RO2-R. + #.065 RO2-N. + #.935 RCHO + #.935 ACET + #-1 XC + XN
	2.01e-11	2.01e-11			MBUTENOL + O3P = #.45 RCHO + #.55 MEK + #1.45 XC
2-Methyl-2-Butene-3-ol [AP]	6.35e-11	8.20e-12	-1.21		MBUTENOL + HO. = #.935 RO2-R. + #.065 RO2-N. + #.311 HCHO + #.624 CCHO + #.624 ACET + #.246 XC + #.311 PRD1
	9.30e-18	9.30e-18			MBUTENOL + O3 = #.099 HO. + #.099 HO2. + #.365 CO + #.091 CO2 + #.3 HCHO + #.015 ACET + #.259 HCOOH + #.285 RCO-OH + #.985 XC + #.7 PRD1
	1.20e-14	4.60e-14	0.80		MBUTENOL + NO3 = #.935 RO2-R. + #.065 RO2-N. + #.935 ACET + #-1 XC + #.935 PRD2 + XN
	2.01e-11	2.01e-11			MBUTENOL + O3P = #.55 MEK + #1.45 XC + #.45 PRD3
	1.97e-11	1.97e-11			PRD1 + HO. = #.017 RO2-R. + #.001 RO2-N. + #.983 RCO-O2. + #.017 HCHO + #.017 MGLY + #-0.019 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + ACET + #-1 XC
	1.93e-11	1.93e-11			PRD2 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD2 + HV = NO2 + HO2. + CO + HCHO + XC
	2.06e-11	2.06e-11			PRD3 + HO. = #.055 RO2-R. + #.004 RO2-N. + #.001 R2O2. + #.942 RCO-O2. + #.015 HCHO + #.015 RCHO + #.04 ACET + #.04 GLY + #-0.106 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = HO2. + #.93 RO2-R. + #.07 RO2-N. + CO + #.93 HCHO + #.93 ACET + #-2.14 XC
Ethyl Acrylate [LP]	2.84e-11	2.84e-11			ET-ACRYL + HO. = #.511 RO2-R. + #.095 RO2-N. + #.864 R2O2. + #.394 CCO-O2. + #.416 HCHO + #.409 PROD2 + #.416 MGLY + #.08 BACL + #-0.795 XC
	1.01e-17	1.01e-17			ET-ACRYL + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.5 MGLY + #.185 HCOOH + #2.5 XC
	2.76e-18	2.76e-18			ET-ACRYL + NO3 = #.172 RO2-R. + #.12 RO2-N. + #1.554 R2O2. + #.708 CCO-O2. + #.145 BACL + #.735 RNO3 + #-2.126 XC + #.265 XN
	4.60e-12	4.60e-12			ET-ACRYL + O3P = #.45 RCHO + #.55 MEK + #1.45 XC
Ethyl Acrylate [AP]	2.84e-11	2.84e-11			ET-ACRYL + HO. = #.511 RO2-R. + #.095 RO2-N. + #.864 R2O2. + #.394 CCO-O2. + #.416 HCHO + #-0.795 XC + #.08 PRD1 + #.416 PRD2 + #.409 PRD3
	1.01e-17	1.01e-17			ET-ACRYL + O3 = #.06 HO. + #.06 HO2. + #.25 CO + #.065 CO2 + #.5 HCHO + #.185 HCOOH + #2.5 XC + #.5 PRD2
	2.76e-18	2.76e-18			ET-ACRYL + NO3 = #.172 RO2-R. + #.12 RO2-N. + #1.554 R2O2. + #.708 CCO-O2. + #.735 RNO3 + #-2.126 XC + #.145 PRD4 + #.265 XN
	4.60e-12	4.60e-12			ET-ACRYL + O3P = #.55 MEK + #1.45 XC + #.45 PRD5
	8.33e-12	8.33e-12			PRD1 + HO. = #.545 HO2. + #.209 RO2-R. + #.015 RO2-N. + #.182 CCO-O2. + #.05 RCO-O2. + #.05 HCHO + #.426 MGLY + #.51 BACL + #.033 XC
		PF=BACL_ADJ			PRD1 + HV = #2 RCO-O2. + #-2 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	6.56e-12	6.56e-12			PRD2 + HO. = #.033 RO2-R. + #.01 RO2-N. + #.212 R2O2. + #.212 CCO-O2. + #.745 RCO-O2. + #.245 MGLY + #-0.454 XC
		PF=MGLY_ADJ			PRD2 + HV = HO2. + RCO-O2. + CO + #-1 XC
	1.96e-11	1.96e-11			PRD3 + HO. = HO2. + #.001 CO2 + #.018 HCHO + #.001 CCHO + #.654 RCHO + #.018 MGLY + #.328 BACL + #2.654 XC
	5.35e-12	5.35e-12			PRD4 + HO. = #.01 NO2 + #.375 HO2. + #.082 RO2-R. + #.039 RO2-N. + #.487 R2O2. + #.493 CCO-O2. + #.001 HCHO + #.01 MGLY + #.95 BACL + #-1.055 XC + #.99 XN
		PF=BACL_ADJ			PRD4 + HV = #2 RCO-O2. + #-2 XC + XN
	2.11e-11	2.11e-11			PRD5 + HO. = #.003 RO2-R. + #.006 RO2-N. + #.082 R2O2. + #.073 CCO-O2. + #.918 RCO-O2. + #.076 RCHO + #.001 MGLY + #-0.164 XC
	3.80e-15	3.80e-15			PRD5 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD5 + HV = #.544 HO2. + #1.191 RO2-R. + #.049 RO2-N. + #.216 CCO-O2. + CO + #.008 MEK + #.726 MGLY + #.216 RCO-OH + #-1.589 XC
Methyl Methacrylate	5.21e-11	5.21e-11			ME-MACRT + HO. = #.935 RO2-R. + #.065 RO2-N. + #.935 HCHO + #.935 BACL + #-0.065 XC
	1.18e-17	1.18e-17			ME-MACRT + O3 = #.707 HO. + #.313 RO2-R. + #.026 RO2-N. + #.327 R2O2. + #.367 RCO-O2. + #.167 CO + #.043 CO2 + #1.034 HCHO + #.273 MGLY + #.333 BACL + #.123 HCOOH + #.221 XC
	6.64e-17	6.64e-17			ME-MACRT + NO3 = #.256 RO2-R. + #.083 RO2-N. + #.935 R2O2. + #.661 RCO-O2. + #.101 CO + #.101 RNO3 + #1.815 XC + #.899 XN
	1.42e-11	1.42e-11			ME-MACRT + O3P = #.4 RCHO + #.6 MEK + #1.4 XC
Butyl Methacrylate	5.21e-11	5.21e-11			BU-MACRT + HO. = #.762 RO2-R. + #.194 RO2-N. + #.164 R2O2. + #.044 RCO-O2. + #.736 HCHO + #.003 RCHO + #.003 MEK + #.068 PROD2 + #.736 BACL + #2.6 XC
	1.18e-17	1.18e-17			BU-MACRT + O3 = #.707 HO. + #.286 RO2-R. + #.09 RO2-N. + #.291 R2O2. + #.331 RCO-O2. + #.167 CO + #.043 CO2 + #.997 HCHO + #.246 MGLY + #.333 BACL + #.123 HCOOH + #3.066 XC
	6.64e-17	6.64e-17			BU-MACRT + NO3 = #.225 RO2-R. + #.346 RO2-N. + #1.446 R2O2. + #.429 RCO-O2. + #.024 RCHO + #.575 RNO3 + #1.115 XC + #.425 XN
	1.42e-11	1.42e-11			BU-MACRT + O3P = #.4 RCHO + #.6 MEK + #4.4 XC
Isobutyl Methacrylate	5.21e-11	5.21e-11			IBUMACRT + HO. = #.795 RO2-R. + #.192 RO2-N. + #.166 R2O2. + #.013 RCO-O2. + #.736 HCHO + #.059 ACET + #.062 MEK + #.013 PROD2 + #.736 BACL + #2.626 XC
	1.18e-17	1.18e-17			IBUMACRT + O3 = #.707 HO. + #.286 RO2-R. + #.09 RO2-N. + #.291 R2O2. + #.331 RCO-O2. + #.167 CO + #.043 CO2 + #.997 HCHO + #.246 MGLY + #.333 BACL + #.123 HCOOH + #3.066 XC
	6.64e-17	6.64e-17			IBUMACRT + NO3 = #.503 RO2-R. + #.328 RO2-N. + #1.464 R2O2. + #.169 RCO-O2. + #.503 ACET + #.113 RNO3 + #3.337 XC + #.887 XN
	1.42e-11	1.42e-11			IBUMACRT + O3P = #.4 RCHO + #.6 MEK + #4.4 XC
Acetaldehyde	1.58e-11	5.60e-12	-0.62		ACETALD + HO. = CCO-O2.
	2.73e-15	1.40e-12	3.70		ACETALD + NO3 = CCO-O2. + XN
		PF=CCHO_R			ACETALD + HV = HO2. + C-O2. + CO
Propionaldehyde	2.00e-11	2.00e-11			PROPALD + HO. = #.034 RO2-R. + #.002 RO2-N. + #.965 RCO-O2. + #.034 CO + #.034 CCHO + #-0.005 XC
	3.80e-15	3.80e-15			PROPALD + NO3 = RCO-O2. + XN
		PF=C2CHO			PROPALD + HV = HO2. + RO2-R. + CO + CCHO
2-Methyl-propanal	2.63e-11	6.61e-12	-0.82		2MEC3AL + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #.91 XC
	3.80e-15	3.80e-15			2MEC3AL + NO3 = RCO-O2. + XC + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			2MEC3AL + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-0.12 XC
Butanal [LP]	2.35e-11	5.26e-12	-0.89		1C4RCHO + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #.924 XC
	3.80e-15	3.80e-15			1C4RCHO + NO3 = RCO-O2. + XC + XN
		PF=C2CHO			1C4RCHO + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-0.06 XC
Butanal [AP]	2.35e-11	5.26e-12	-0.89		1C4RCHO + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.038 RCHO + #.001 GLY + #.924 XC + #.035 PRD1
	3.80e-15	3.80e-15			1C4RCHO + NO3 = RCO-O2. + XC + XN
		PF=C2CHO			1C4RCHO + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-0.06 XC
	6.11e-11	6.11e-11			PRD1 + HO. = RCO-O2.
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = RO2-R. + CCO-O2. + CO + HCHO + #-1 XC
2,2-Dimethy-lpropanal (pivaldehyde)	2.66e-11	6.82e-12	-0.81		22DMC3AL + HO. = #.023 RO2-R. + #.003 RO2-N. + #.024 R2O2. + #.974 RCO-O2. + #.023 CO + #.024 HCHO + #.001 RCHO + #.023 ACET + #1.946 XC
	3.80e-15	3.80e-15			22DMC3AL + NO3 = RCO-O2. + #2 XC + XN
		PF=C2CHO			22DMC3AL + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 TBU-O. + CO + #.882 XC
3-Methylbutanal (Isovaleraldehyde) [LP]	2.74e-11	2.74e-11			3MC4RCHO + HO. = #.129 RO2-R. + #.012 RO2-N. + #.112 R2O2. + #.002 C-O2. + #.856 RCO-O2. + #.125 CO + #.092 HCHO + #.036 RCHO + #.096 ACET + #.004 GLY + #1.736 XC
	3.80e-15	3.80e-15			3MC4RCHO + NO3 = RCO-O2. + #2 XC + XN
		PF=C2CHO			3MC4RCHO + HV = #.652 HO2. + #1.294 RO2-R. + #.053 RO2-N. + CO + #.348 HCHO + #.613 RCHO + #.334 ACET + #.492 XC
3-Methylbutanal (Isovaleraldehyde) [AP]	2.74e-11	2.74e-11			3MC4RCHO + HO. = #.129 RO2-R. + #.012 RO2-N. + #.112 R2O2. + #.002 C-O2. + #.856 RCO-O2. + #.125 CO + #.092 HCHO + #.096 ACET + #.004 GLY + #1.736 XC + #.036 PRD1
	3.80e-15	3.80e-15			3MC4RCHO + NO3 = RCO-O2. + #2 XC + XN
		PF=C2CHO			3MC4RCHO + HV = #.652 HO2. + #1.294 RO2-R. + #.053 RO2-N. + CO + #.348 HCHO + #.334 ACET + #.492 XC + #.613 PRD2
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	2.60e-11	2.60e-11			PRD2 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
Pentanal (Valeraldehyde) [LP]	2.85e-11	6.34e-12	-0.89		1C5RCHO + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.087 RCHO + #.002 MGLY + #1.851 XC
	3.80e-15	3.80e-15			1C5RCHO + NO3 = RCO-O2. + #2 XC + XN
		PF=C2CHO			1C5RCHO + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.931 RCHO + #.792 XC
Pentanal (Valeraldehyde) [AP]	2.85e-11	6.34e-12	-0.89		1C5RCHO + HO. = #.089 RO2-R. + #.018 RO2-N. + #.08 R2O2. + #.893 RCO-O2. + #.043 CO + #.011 HCHO + #.021 CCHO + #.012 RCHO + #.002 MGLY + #1.851 XC + #.075 PRD1

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15 PF=C2CHO			1C5RCHO + NO3 = RCO-O2. + #2 XC + XN 1C5RCHO + HV = #.245 HO2. + #1.686 RO2-R. + #.069 RO2-N. + CO + #.792 XC + #.931 PRD2
	2.33e-11	2.33e-11			PRD1 + HO. = #.088 RO2-R. + #.008 RO2-N. + #.015 R2O2. + #.905 RCO-O2. + #.052 CO + #.014 HCHO + #.015 CCHO + #.073 RCHO + #.001 GLY + #-0.076 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = HO2. + #.98 RO2-R. + #.02 RO2-N. + CO + #.98 RCHO + #-1.06 XC
	2.52e-11	2.52e-11			PRD2 + HO. = #.122 HO2. + #.086 RO2-R. + #.004 RO2-N. + #.003 R2O2. + #.787 RCO-O2. + #.037 CO + #.045 HCHO + #.003 CCHO + #.206 RCHO + #-0.092 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.99 HO2. + #1.005 RO2-R. + #.004 RO2-N. + CO + #.026 HCHO + #.002 CCHO + #.986 RCHO + #-1.013 XC
Glutaraldehyde	4.16e-11	4.16e-11			GLTRALD + HO. = #.04 RO2-R. + #.009 RO2-N. + #.051 R2O2. + #.951 RCO-O2. + #.033 CO + #.023 HCHO + #.04 RCHO + #.001 GLY + #1.915 XC
	7.60e-15	7.60e-15 PF=C2CHO			GLTRALD + NO3 = RCO-O2. + #2 XC + XN GLTRALD + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 RCO-O2. + CO + #.882 XC
Hexanal [LP]	2.43e-11	2.43e-11			1C6RCHO + HO. = #.112 RO2-R. + #.04 RO2-N. + #.154 R2O2. + #.848 RCO-O2. + #.014 CO + #.002 HCHO + #.103 RCHO + #.018 MGLY + #2.834 XC
	3.80e-15	3.80e-15 PF=C2CHO			1C6RCHO + NO3 = RCO-O2. + #3 XC + XN 1C6RCHO + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.874 RCHO + #1.623 XC
Hexanal [AP]	2.43e-11	2.43e-11			1C6RCHO + HO. = #.112 RO2-R. + #.04 RO2-N. + #.154 R2O2. + #.848 RCO-O2. + #.014 CO + #.002 HCHO + #.009 RCHO + #.018 MGLY + #2.834 XC + #.094 PRD1
	3.80e-15	3.80e-15 PF=C2CHO			1C6RCHO + NO3 = RCO-O2. + #3 XC + XN 1C6RCHO + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #1.623 XC + #.874 PRD2
	4.90e-11	4.90e-11			PRD1 + HO. = #.115 HO2. + #.118 RO2-R. + #.013 RO2-N. + #.015 CCO-O2. + #.739 RCO-O2. + #.027 HCHO + #.143 RCHO + #.071 GLY + #.11 MGLY + #-0.251 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD1 + NO3 = RCO-O2. + XN PRD1 + HV = #1.122 HO2. + #.424 RO2-R. + #.029 RO2-N. + #.424 RCO-O2. + CO + #.424 HCHO + #.546 RCHO + #-1.513 XC
	3.01e-11	3.01e-11			PRD2 + HO. = #.276 HO2. + #.074 RO2-R. + #.005 RO2-N. + #.645 RCO-O2. + #.025 CO + #.045 CCHO + #.348 RCHO + #.001 MGLY + #-0.13 XC
	3.80e-15	3.80e-15 PF=C2CHO			PRD2 + NO3 = RCO-O2. + XN PRD2 + HV = #.215 HO2. + #1.715 RO2-R. + #.07 RO2-N. + CO + #.93 RCHO + #-1.211 XC
Heptanal [LP]	2.57e-11	2.57e-11			1C7RCHO + HO. = #.136 RO2-R. + #.067 RO2-N. + #.191 R2O2. + #.797 RCO-O2. + #.009 CO + #.118 RCHO + #.017 MGLY + #3.79 XC
	3.80e-15	3.80e-15 PF=C2CHO			1C7RCHO + NO3 = RCO-O2. + #4 XC + XN 1C7RCHO + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.814 RCHO + #2.443 XC
Heptanal [AP]	2.57e-11	2.57e-11			1C7RCHO + HO. = #.136 RO2-R. + #.067 RO2-N. + #.191 R2O2. + #.797 RCO-O2. + #.009 CO + #.017 MGLY + #3.79 XC + #.118 PRD1
	3.80e-15	3.80e-15 PF=C2CHO			1C7RCHO + NO3 = RCO-O2. + #4 XC + XN 1C7RCHO + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #2.443 XC + #.814 PRD2

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	4.87e-11	4.87e-11			PRD1 + HO. = #.156 HO2. + #.132 RO2-R. + #.021 RO2-N. + #.009 CCO-O2. + #.683 RCO-O2. + #.001 CO + #.025 CCHO + #.269 RCHO + #.043 GLY + #.067 MGLY + #-0.34 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.911 HO2. + #.642 RO2-R. + #.069 RO2-N. + #.052 CCO-O2. + #.325 RCO-O2. + CO + #.532 HCHO + #.605 RCHO + #-1.845 XC
	3.32e-11	3.32e-11			PRD2 + HO. = #.278 HO2. + #.124 RO2-R. + #.013 RO2-N. + #.585 RCO-O2. + #.009 CO + #.017 CCHO + #.427 RCHO + #.013 MGLY + #-0.199 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.077 CCHO + #.874 RCHO + #-1.531 XC
Octanal [LP]	2.71e-11	2.71e-11			1C8RCHO + HO. = #.164 RO2-R. + #.096 RO2-N. + #.219 R2O2. + #.74 RCO-O2. + #.008 CO + #.149 RCHO + #.015 MGLY + #4.704 XC
	3.80e-15	3.80e-15			1C8RCHO + NO3 = RCO-O2. + #5 XC + XN
		PF=C2CHO			1C8RCHO + HV = #.135 HO2. + #1.613 RO2-R. + #.252 RO2-N. + CO + #.748 RCHO + #3.244 XC
Octanal [AP]	2.71e-11	2.71e-11			1C8RCHO + HO. = #.164 RO2-R. + #.096 RO2-N. + #.219 R2O2. + #.74 RCO-O2. + #.008 CO + #.015 MGLY + #4.704 XC + #.149 PRD1
	3.80e-15	3.80e-15			1C8RCHO + NO3 = RCO-O2. + #5 XC + XN
		PF=C2CHO			1C8RCHO + HV = #.135 HO2. + #1.613 RO2-R. + #.252 RO2-N. + CO + #3.244 XC + #.748 PRD2
	4.80e-11	4.80e-11			PRD1 + HO. = #.149 HO2. + #.174 RO2-R. + #.036 RO2-N. + #.004 CCO-O2. + #.636 RCO-O2. + #.001 CO + #.005 HCHO + #.011 CCHO + #.367 RCHO + #.027 GLY + #.046 MGLY + #-0.457 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.739 HO2. + #.846 RO2-R. + #.132 RO2-N. + #.282 RCO-O2. + CO + #.423 HCHO + #.677 RCHO + #-2.094 XC
	3.46e-11	3.46e-11			PRD2 + HO. = #.235 HO2. + #.176 RO2-R. + #.028 RO2-N. + #.561 RCO-O2. + #.006 CO + #.479 RCHO + #.013 MGLY + #-0.331 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.898 RCHO + #-1.807 XC
Acrolein [LP]	1.99e-11	1.99e-11			ACROLEIN + HO. = #.25 RO2-R. + #.75 MA-RCO3. + #.167 CO + #.083 HCHO + #.167 CCHO + #.083 GLY + #-0.75 XC
	2.90e-19	1.36e-15	5.01		ACROLEIN + O3 = #.31 HO. + #.81 HO2. + CO + #.315 CO2 + #.5 HCHO + #.5 GLY + #.185 HCOOH
	2.94e-15	2.94e-15			ACROLEIN + NO3 = #.031 RO2-R. + #.002 RO2-N. + #.967 MA-RCO3. + #.031 CO + #.031 RCHO + #-1.003 XC + XN
	2.37e-12	2.37e-12			ACROLEIN + O3P = RCHO
		PF=ACROLEIN QY = 2.0e-3			ACROLEIN + HV = #.172 HO. + #1.01 HO2. + #.172 C-O2. + #.33 MA-RCO3. + #1.182 CO + #.046 CO2 + #.34 HCHO + #.112 CCO-OH + #.046 INERT + #-0.284 XC
Acrolein [AP]	1.99e-11	1.99e-11			ACROLEIN + HO. = #.25 RO2-R. + #.75 MA-RCO3. + #.167 CO + #.083 HCHO + #.167 CCHO + #.083 GLY + #-0.75 XC
	2.90e-19	1.36e-15	5.01		ACROLEIN + O3 = #.31 HO. + #.81 HO2. + CO + #.315 CO2 + #.5 HCHO + #.5 GLY + #.185 HCOOH
	2.94e-15	2.94e-15			ACROLEIN + NO3 = #.031 RO2-R. + #.002 RO2-N. + #.967 MA-RCO3. + #.031 CO + #-1.003 XC + #.031 PRD1 + XN
	2.37e-12	2.37e-12			ACROLEIN + O3P = PRD2
		PF=ACROLEIN QY = 2.0e-3			ACROLEIN + HV = #.172 HO. + #1.01 HO2. + #.172 C-O2. + #.33 MA-RCO3. + #1.182 CO + #.046 CO2 + #.34 HCHO + #.112 CCO-OH + #.046 INERT + #-0.284 XC
	1.93e-11	1.93e-11			PRD1 + HO. = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD1 + HV = NO2 + HO2. + CO + HCHO + XC
	2.84e-11	2.84e-11			PRD2 + HO. = #.014 RO2-R. + #.009 R2O2. + #.986 RCO-O2. + #.008 CO + #.005 GLY + #.009 MGLY + #-0.004 XC
	5.51e-15	5.51e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.45 HO2. + #1.55 RO2-R. + #1.657 CO + #.039 CO2 + #.47 HCHO + #.019 GLY + #.226 HCOOH + #.285 XC
Crotonaldehyde [LP]	3.64e-11	3.64e-11			CROTALD + HO. = #.528 RO2-R. + #.022 RO2-N. + #.45 MA-RCO3. + #.032 CO + #.497 CCHO + #.032 RCHO + #.497 GLY + #-0.043 XC
	9.00e-19	9.00e-19			CROTALD + O3 = #.51 HO. + #.75 HO2. + #.26 C-O2. + #1.01 CO + #.32 CO2 + #.5 CCHO + #.5 GLY + #.17 CCO-OH + #.07 INERT + #.07 XC
	5.12e-15	5.12e-15			CROTALD + NO3 = #.129 NO2 + #.376 RO2-R. + #.044 RO2-N. + #.129 R2O2. + #.45 MA-RCO3. + #.253 CO + #.45 HNO3 + #.129 CCHO + #.376 RCHO + #.129 GLY + #.035 XC + #.421 XN
	7.29e-12	7.29e-12			CROTALD + O3P = #.88 RCHO + #.12 MGLY + XC
		PF=ACROLEIN QY = 4.1e-3			CROTALD + HV = #2 HO2. + #2 CO + CCHO
Crotonaldehyde [AP]	3.64e-11	3.64e-11			CROTALD + HO. = #.528 RO2-R. + #.022 RO2-N. + #.45 MA-RCO3. + #.032 CO + #.497 CCHO + #.497 GLY + #-0.043 XC + #.032 PRD1
	9.00e-19	9.00e-19			CROTALD + O3 = #.51 HO. + #.75 HO2. + #.26 C-O2. + #1.01 CO + #.32 CO2 + #.5 CCHO + #.5 GLY + #.17 CCO-OH + #.07 INERT + #.07 XC
	5.12e-15	5.12e-15			CROTALD + NO3 = #.129 NO2 + #.376 RO2-R. + #.044 RO2-N. + #.129 R2O2. + #.45 MA-RCO3. + #.253 CO + #.45 HNO3 + #.129 CCHO + #.129 GLY + #.035 XC + #.376 PRD2 + #.421 XN
	7.29e-12	7.29e-12			CROTALD + O3P = XC + #.88 PRD3 + #.12 PRD4
		PF=ACROLEIN QY = 4.1e-3			CROTALD + HV = #2 HO2. + #2 CO + CCHO
	2.46e-11	2.46e-11			PRD1 + HO. = #.209 HO2. + #.791 RCO-O2. + #.209 MGLY + #-0 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + CCHO
	3.30e-11	3.30e-11			PRD2 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD2 + HV = NO2 + HO2. + CO + #.672 CCHO + #.328 MGLY + #-0.328 XC
	2.57e-11	2.57e-11			PRD3 + HO. = #.016 RO2-R. + #.002 RO2-N. + #.04 R2O2. + #.011 CCO-O2. + #.97 RCO-O2. + #.016 CO + #.012 MGLY + #-0.014 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #1.087 RO2-R. + #.776 R2O2. + #.913 CCO-O2. + CO + #.063 CO2 + #.136 HCHO + #.063 CCHO + #.776 HCOOH + #-0.951 XC
	1.30e-11	1.30e-11			PRD4 + HO. = #.035 RO2-R. + #.004 RO2-N. + #.057 R2O2. + #.961 RCO-O2. + #.001 HCHO + #.052 CCHO + #.035 MGLY + #-0.117 XC
	2.53e-15	2.53e-15			PRD4 + NO3 = RCO-O2. + XN
		PF=MGLY_ADJ			PRD4 + HV = HO2. + RCO-O2. + CO + #-1 XC
Methacrolein [LP]	3.35e-11	1.86e-11	-0.35		METHACRO + HO. = #.48 RO2-R. + #.02 RO2-N. + #.5 MA-RCO3. + #.396 CO + #.084 HCHO + #.396 MEK + #.084 MGLY + #-0.436 XC
	1.13e-18	1.36e-15	4.20		METHACRO + O3 = #.208 HO. + #.008 HO2. + #.1 RO2-R. + #.1 RCO-O2. + #.45 CO + #.117 CO2 + #.2 HCHO + #.9 MGLY + #.333 HCOOH + #-0.1 XC
	4.58e-15	1.50e-12	3.43		METHACRO + NO3 = #.48 RO2-R. + #.02 RO2-N. + #.5 MA-RCO3. + #.48 CO + #.5 HNO3 + #1.401 XC + #.5 XN
	6.19e-12	6.19e-12			METHACRO + O3P = RCHO + XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	PF=ACROLEIN QY = 4.1e-3				METHACRO + HV = #.33 HO. + #.34 HO2. + #.33 RO2-R. + #.67 CCO-O2. + #.33 MA-RCO3. + #.67 CO + #.67 HCHO + #-0 XC
Methacrolein [AP]	3.35e-11	1.86e-11	-0.35		METHACRO + HO. = #.48 RO2-R. + #.02 RO2-N. + #.5 MA-RCO3. + #.396 CO + #.084 HCHO + #.396 MEK + #.084 MGLY + #-0.436 XC
	1.13e-18	1.36e-15	4.20		METHACRO + O3 = #.208 HO. + #.008 HO2. + #.1 RO2-R. + #.1 RCO-O2. + #.45 CO + #.117 CO2 + #.2 HCHO + #.9 MGLY + #.333 HCOOH + #-0.1 XC
	4.58e-15	1.50e-12	3.43		METHACRO + NO3 = #.48 RO2-R. + #.02 RO2-N. + #.5 MA-RCO3. + #.48 CO + #.5 HNO3 + #1.401 XC + #.5 XN
	6.19e-12	6.19e-12			METHACRO + O3P = XC + PRD1
	PF=ACROLEIN QY = 4.1e-3				METHACRO + HV = #.33 HO. + #.34 HO2. + #.33 RO2-R. + #.67 CCO-O2. + #.33 MA-RCO3. + #.67 CO + #.67 HCHO + #-0 XC
	2.76e-11	2.76e-11			PRD1 + HO. = #.011 RO2-R. + #.989 RCO-O2. + #.011 CO + #.011 MGLY + #-0.012 XC
	5.32e-15	5.32e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.4 HO2. + #1.571 RO2-R. + #.029 RO2-N. + #1.601 CO + #.38 CCHO + #.221 CCO-OH + #-0.348 XC
Hydroxy Methacrolein [LP]	4.30e-11	4.30e-11			HOMACR + HO. = #.596 RO2-R. + #.024 RO2-N. + #.38 MA-RCO3. + #.444 CO + #.151 HCHO + #.444 PROD2 + #.151 MGLY + #-1.382 XC
	1.13e-18	1.36e-15	4.20		HOMACR + O3 = #.208 HO. + #.208 HO2. + #.45 CO + #.117 CO2 + #.1 HCHO + MGLY + #.333 HCOOH
	4.58e-15	1.50e-12	3.43		HOMACR + NO3 = #.48 RO2-R. + #.02 RO2-N. + #.5 MA-RCO3. + #.452 CO + #.5 HNO3 + #.028 HCHO + #.028 MGLY + #.452 RNO3 + #-1.396 XC + #.048 XN
	9.95e-12	9.95e-12			HOMACR + O3P = RCHO + XC
	PF=ACROLEIN QY = 4.1e-3				HOMACR + HV = HO2. + RCO-O2. + CO + HCHO + #-1 XC
Hydroxy Meth-acrolein [AP]	4.30e-11	4.30e-11			HOMACR + HO. = #.596 RO2-R. + #.024 RO2-N. + #.38 MA-RCO3. + #.444 CO + #.151 HCHO + #-1.382 XC + #.151 PRD1 + #.444 PRD2
	1.13e-18	1.36e-15	4.20		HOMACR + O3 = #.208 HO. + #.208 HO2. + #.45 CO + #.117 CO2 + #.1 HCHO + #.333 HCOOH + PRD3
	4.58e-15	1.50e-12	3.43		HOMACR + NO3 = #.48 RO2-R. + #.02 RO2-N. + #.5 MA-RCO3. + #.452 CO + #.5 HNO3 + #.028 HCHO + #.452 RNO3 + #-1.396 XC + #.028 PRD4 + #.048 XN
	9.95e-12	9.95e-12			HOMACR + O3P = XC + PRD5
	PF=ACROLEIN QY = 4.1e-3				HOMACR + HV = HO2. + RCO-O2. + CO + HCHO + #-1 XC
	1.48e-11	1.48e-11			PRD1 + HO. = #.166 HO2. + #.834 RCO-O2. + #.037 HCHO + #.166 MGLY + #-0.037 XC
	2.53e-15	2.53e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=MGLY_ADJ			PRD1 + HV = HO2. + RCO-O2. + CO + #-1 XC
	6.01e-12	6.01e-12			PRD2 + HO. = #.817 HO2. + #.183 RCO-O2. + #.183 HCHO + #.817 MGLY + #2.817 XC
	PF=KETONE QY = 1.0e-1				PRD2 + HV = HO2. + RCO-O2. + HCHO + #2 XC
	1.56e-11	1.56e-11			PRD3 + HO. = #.15 HO2. + #.85 RCO-O2. + #.034 HCHO + #.15 MGLY + #-0.034 XC
	2.78e-15	2.78e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=MGLY_ADJ			PRD3 + HV = HO2. + RCO-O2. + CO + #-1 XC
	1.18e-11	1.18e-11			PRD4 + HO. = RCO-O2. + XN
	2.53e-15	2.53e-15			PRD4 + NO3 = RCO-O2. + #2 XN
		PF=MGLY_ADJ			PRD4 + HV = HO2. + RCO-O2. + CO + #-1 XC + XN
	3.18e-11	3.18e-11			PRD5 + HO. = #.14 HO2. + #.012 RO2-R. + #.847 RCO-O2. + #.011 CO + #.14 RCHO + #.012 MGLY + #-0.013 XC
	5.32e-15	5.32e-15			PRD5 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD5 + HV = #.4 HO2. + #1.6 RO2-R. + #1.578 CO + #.007 HCHO + #.393 CCHO + #.285 MEK + #.007 GLY + #.13 MGLY + #.185 RCO-OH + #-1.47 XC
Acetone	2.19e-13	2.80e-12	1.51		ACETONE + HO. = R2O2. + CCO-O2. + HCHO
		PF=ACETONE			ACETONE + HV = C-O2. + CCO-O2.
Cyclobutanone	8.70e-13	8.70e-13			CC4-KET + HO. = #.073 RO2-N. + #1.782 R2O2. + #.927 RCO-O2. + #.821 HCHO + #-0.041 XC
		PF=KETONE QY = 1.5e-1			CC4-KET + HV = #4 XC
Methyl Ethyl Ketone [LP]	1.19e-12	1.30e-12	0.05		MEK + HO. = #.376 RO2-R. + #.039 RO2-N. + #.591 R2O2. + #.51 CCO-O2. + #.074 RCO-O2. + #.088 HCHO + #.504 CCHO + #.376 RCHO + #.297 XC
		PF=KETONE QY = 1.5e-1			MEK + HV = RO2-R. + CCO-O2. + CCHO
Methyl Ethyl Ketone [AP]	1.19e-12	1.30e-12	0.05		MEK + HO. = #.376 RO2-R. + #.039 RO2-N. + #.591 R2O2. + #.51 CCO-O2. + #.074 RCO-O2. + #.088 HCHO + #.504 CCHO + #.297 XC + #.376 PRD1
		PF=KETONE QY = 1.5e-1			MEK + HV = RO2-R. + CCO-O2. + CCHO
	6.11e-11	6.11e-11			PRD1 + HO. = RCO-O2.
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = RO2-R. + CCO-O2. + CO + HCHO + #-1 XC
Cyclopentanone [LP]	2.94e-12	2.94e-12			CC5-KET + HO. = #.624 RO2-R. + #.118 RO2-N. + #1.072 R2O2. + #.258 RCO-O2. + #.077 HCHO + #.624 RCHO + #.029 GLY + #1.512 XC
		PF=KETONE QY = 1.0e-1			CC5-KET + HV = #5 XC
Cyclopentanone [AP]	2.94e-12	2.94e-12			CC5-KET + HO. = #.624 RO2-R. + #.118 RO2-N. + #1.072 R2O2. + #.258 RCO-O2. + #.077 HCHO + #.029 GLY + #1.512 XC + #.624 PRD1
		PF=KETONE QY = 1.0e-1			CC5-KET + HV = #5 XC
	1.22e-10	1.22e-10			PRD1 + HO. = RCO-O2.
	7.60e-15	7.60e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 RCO-O2. + CO + #.961 HCHO + #-2.079 XC
2-Pentanone [LP]	4.56e-12	4.56e-12			MPK + HO. = #.154 RO2-R. + #.065 RO2-N. + #1.373 R2O2. + #.761 CCO-O2. + #.02 RCO-O2. + #.612 HCHO + #.591 CCHO + #.203 RCHO + #.12 MEK + #.142 XC
		PF=KETONE QY = 1.0e-1			MPK + HV = #.98 RO2-R. + #.02 RO2-N. + CCO-O2. + #.98 RCHO + #-0.06 XC
2-Pentanone [AP]	4.56e-12	4.56e-12			MPK + HO. = #.154 RO2-R. + #.065 RO2-N. + #1.373 R2O2. + #.761 CCO-O2. + #.02 RCO-O2. + #.612 HCHO + #.591 CCHO + #.17 RCHO + #.12 MEK + #.142 XC + #.033 PRD1
		PF=KETONE QY = 1.0e-1			MPK + HV = #.98 RO2-R. + #.02 RO2-N. + CCO-O2. + #.98 RCHO + #-0.06 XC
	2.29e-11	2.29e-11			PRD1 + HO. = #.112 RO2-R. + #.01 RO2-N. + #.036 R2O2. + #.036 CCO-O2. + #.842 RCO-O2. + #.112 CO + #.148 RCHO + #-0.214 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.967 HO2. + #.977 RO2-R. + #.039 RO2-N. + #.017 CCO-O2. + CO + #.033 HCHO + #.944 RCHO + #-1.135 XC
3-Pentanone [LP]	2.00e-12	2.00e-12			DEK + HO. = #.375 RO2-R. + #.067 RO2-N. + #.588 R2O2. + #.559 RCO-O2. + #.559 CCHO + #.375 RCHO + #.682 XC
		PF=KETONE QY = 1.0e-1			DEK + HV = RO2-R. + RCO-O2. + CCHO
3-Pentanone [AP]	2.00e-12	2.00e-12			DEK + HO. = #.375 RO2-R. + #.067 RO2-N. + #.588 R2O2. + #.559 RCO-O2. + #.559 CCHO + #.682 XC + #.375 PRD1
		PF=KETONE QY = 1.0e-1			DEK + HV = RO2-R. + RCO-O2. + CCHO
	6.23e-11	6.23e-11			PRD1 + HO. = #.001 RO2-N. + #.011 R2O2. + #.999 RCO-O2. + #.011 CCHO + #-0.024 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.039 HO2. + #.961 RO2-R. + #.039 RO2-N. + #.961 RCO-O2. + CO + #.961 HCHO + #-2.079 XC
Cyclohexanone [LP]	6.39e-12	6.39e-12			CC6-KET + HO. = #.386 RO2-R. + #.178 RO2-N. + #.722 R2O2. + #.436 RCO-O2. + #.059 HCHO + #.194 RCHO + #.197 PROD2 + #1.802 XC
		PF=KETONE QY = 5.0e-2			CC6-KET + HV = #6 XC
Cyclohexanone [AP]	6.39e-12	6.39e-12			CC6-KET + HO. = #.386 RO2-R. + #.178 RO2-N. + #.722 R2O2. + #.436 RCO-O2. + #.059 HCHO + #1.802 XC + #.197 PRD1 + #.194 PRD2
		PF=KETONE QY = 5.0e-2			CC6-KET + HV = #6 XC
	1.52e-11	1.52e-11			PRD1 + HO. = #.124 RO2-R. + #.145 RO2-N. + #1.218 R2O2. + #.731 RCO-O2. + #.44 HCHO + #.124 MEK + #2 XC
		PF=KETONE QY = 5.0e-2			PRD1 + HV = #5.212 XC
	8.38e-11	8.38e-11			PRD2 + HO. = #.03 RO2-R. + #.004 RO2-N. + #.009 R2O2. + #.966 RCO-O2. + #.03 CO + #.039 RCHO + #-0.071 XC
	7.60e-15	7.60e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = #.489 HO2. + #.956 RO2-R. + #.066 RO2-N. + #.488 RCO-O2. + CO + #.468 HCHO + #.446 RCHO + #.02 GLY + #-1.708 XC
4-Methyl-2-Pentanone [LP]	1.41e-11	1.41e-11			MIBK + HO. = #.012 RO2-R. + #.099 RO2-N. + #1.706 R2O2. + #.878 CCO-O2. + #.011 RCO-O2. + #.827 HCHO + #.021 CCHO + #.096 RCHO + #.768 ACET + #.004 MEK + #.135 XC
		PF=KETONE QY = 5.0e-2			MIBK + HV = #.947 RO2-R. + #.053 RO2-N. + #.348 R2O2. + CCO-O2. + #.348 HCHO + #.613 RCHO + #.334 ACET + #.492 XC
4-Methyl-2-Pentanone [AP]	1.41e-11	1.41e-11			MIBK + HO. = #.012 RO2-R. + #.099 RO2-N. + #1.706 R2O2. + #.878 CCO-O2. + #.011 RCO-O2. + #.827 HCHO + #.021 CCHO + #.768 ACET + #.004 MEK + #.135 XC + #.096 PRD1
		PF=KETONE QY = 5.0e-2			MIBK + HV = #.947 RO2-R. + #.053 RO2-N. + #.348 R2O2. + CCO-O2. + #.348 HCHO + #.334 ACET + #.492 XC + #.613 PRD2
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	2.60e-11	2.60e-11			PRD2 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
Methyl n-Butyl Ketone [LP]	9.10e-12	9.10e-12			MNBK + HO. = #.424 RO2-R. + #.102 RO2-N. + #1.014 R2O2. + #.459 CCO-O2. + #.014 RCO-O2. + #.338 HCHO + #.195 CCHO + #.65 RCHO + #.145 MEK + #.088 PROD2 + #.64 XC
		PF=KETONE QY = 5.0e-2			MNBK + HV = #.931 RO2-R. + #.069 RO2-N. + #.755 R2O2. + CCO-O2. + #.931 RCHO + #.792 XC
Methyl n-Butyl Ketone [AP]	9.10e-12	9.10e-12			MNBK + HO. = #.424 RO2-R. + #.102 RO2-N. + #1.014 R2O2. + #.459 CCO-O2. + #.014 RCO-O2. + #.338 HCHO + #.195 CCHO + #.322 RCHO + #.145 MEK + #.64 XC + #.328 PRD1 + #.088 PRD2
		PF=KETONE QY = 5.0e-2			MNBK + HV = #.931 RO2-R. + #.069 RO2-N. + #.755 R2O2. + CCO-O2. + #.792 XC + #.931 PRD3
	4.68e-11	4.68e-11			PRD1 + HO. = #.033 RO2-R. + #.003 RO2-N. + #.006 R2O2. + #.964 RCO-O2. + #.02 CO + #.005 HCHO + #.006 CCHO + #.027 RCHO + #-0.028 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.377 HO2. + #.992 RO2-R. + #.008 RO2-N. + #.623 CCO-O2. + CO + #.623 HCHO + #.369 RCHO + #-1.023 XC
	5.68e-12	5.68e-12			PRD2 + HO. = #.098 RO2-N. + #.902 R2O2. + #.869 CCO-O2. + #.033 RCO-O2. + #.033 HCHO + #.869 RCHO + #.936 XC
		PF=KETONE QY = 5.0e-2			PRD2 + HV = #.944 RO2-R. + #.039 RO2-N. + #.033 R2O2. + #1.017 CCO-O2. + #.033 HCHO + #.944 RCHO + #.865 XC
	2.52e-11	2.52e-11			PRD3 + HO. = #.122 HO2. + #.086 RO2-R. + #.004 RO2-N. + #.003 R2O2. + #.787 RCO-O2. + #.037 CO + #.045 HCHO + #.003 CCHO + #.206 RCHO + #-0.092 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.99 HO2. + #1.005 RO2-R. + #.004 RO2-N. + CO + #.026 HCHO + #.002 CCHO + #.986 RCHO + #-1.013 XC
Methyl t-Butyl Ketone	1.21e-12	1.21e-12			MTBK + HO. = #.021 RO2-R. + #.151 RO2-N. + #1.653 R2O2. + #.772 CCO-O2. + #.055 RCO-O2. + #.881 HCHO + #.021 RCHO + #.772 ACET + #.121 XC
		PF=KETONE QY = 5.0e-2			MTBK + HV = #.039 RO2-N. + #.961 R2O2. + CCO-O2. + #.961 TBU-O. + #.882 XC
2-Heptanone [LP]	1.17e-11	1.17e-11			C7-KET-2 + HO. = #.513 RO2-R. + #.193 RO2-N. + #.936 R2O2. + #.283 CCO-O2. + #.011 RCO-O2. + #.099 HCHO + #.013 CCHO + #.59 RCHO + #.347 PROD2 + #1.265 XC
		PF=KETONE QY = 2.0e-2			C7-KET-2 + HV = #.874 RO2-R. + #.126 RO2-N. + #.935 R2O2. + CCO-O2. + #.874 RCHO + #1.623 XC
2-Heptanone [AP]	1.17e-11	1.17e-11			C7-KET-2 + HO. = #.513 RO2-R. + #.193 RO2-N. + #.936 R2O2. + #.283 CCO-O2. + #.011 RCO-O2. + #.099 HCHO + #.013 CCHO + #.14 RCHO + #1.265 XC + #.449 PRD1 + #.347 PRD2
		PF=KETONE QY = 2.0e-2			C7-KET-2 + HV = #.874 RO2-R. + #.126 RO2-N. + #.935 R2O2. + CCO-O2. + #1.623 XC + #.874 PRD3
	3.85e-11	3.85e-11			PRD1 + HO. = #.069 HO2. + #.056 RO2-R. + #.007 RO2-N. + #.02 R2O2. + #.869 RCO-O2. + #.026 CO + #.005 HCHO + #.019 CCHO + #.12 RCHO + #.001 MGLY + #-0.08 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = #.311 HO2. + #1.323 RO2-R. + #.037 RO2-N. + #.329 CCO-O2. + CO + #.329 HCHO + #.634 RCHO + #-1.11 XC
	8.79e-12	8.79e-12			PRD2 + HO. = #.185 HO2. + #.398 RO2-R. + #.102 RO2-N. + #.266 R2O2. + #.1 CCO-O2. + #.216 RCO-O2. + #.281 HCHO + #.041 CCHO + #.747 RCHO + #.053 MEK + #.047 MGLY + #1.585 XC
		PF=KETONE QY = 1.4e-2			PRD2 + HV = #.189 RO2-R. + #.037 RO2-N. + #.782 R2O2. + #.897 CCO-O2. + #.876 RCO-O2. + #.769 HCHO + #.007 CCHO + #.189 RCHO + #.004 XC
	3.01e-11	3.01e-11			PRD3 + HO. = #.276 HO2. + #.074 RO2-R. + #.005 RO2-N. + #.645 RCO-O2. + #.025 CO + #.045 CCHO + #.348 RCHO + #.001 MGLY + #-0.13 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.215 HO2. + #1.715 RO2-R. + #.07 RO2-N. + CO + #.93 RCHO + #-1.211 XC
2-Methyl-3-Hexanone [LP]	7.21e-12	7.21e-12			2M-3-HXO + HO. = #.298 RO2-R. + #.163 RO2-N. + #.827 R2O2. + #.539 RCO-O2. + #.19 HCHO + #.187 CCHO + #.161 RCHO + #.252 ACET + #.244 MEK + #1.627 XC
		PF=KETONE QY = 2.0e-2			2M-3-HXO + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #.94 XC
2-Methyl-3-Hexanone [AP]	7.21e-12	7.21e-12			2M-3-HXO + HO. = #.298 RO2-R. + #.163 RO2-N. + #.827 R2O2. + #.539 RCO-O2. + #.19 HCHO + #.187 CCHO + #.107 RCHO + #.252 ACET + #.244 MEK + #1.627 XC + #.054 PRD1
		PF=KETONE QY = 2.0e-2			2M-3-HXO + HV = #.98 RO2-R. + #.02 RO2-N. + RCO-O2. + #.98 RCHO + #.94 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	6.68e-11	6.68e-11			PRD1 + HO. = #.029 RO2-R. + #.013 RO2-N. + #.062 R2O2. + #.958 RCO-O2. + #.011 HCHO + #.012 CCHO + #.04 RCHO + #.02 MGLY + #-0.17 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #.902 RO2-R. + #.098 RO2-N. + #.902 RCO-O2. + CO + #.902 CCHO + #-3.098 XC
Di-Isopropyl Ketone [LP]	5.38e-12	5.38e-12			DIPK + HO. = #.095 RO2-R. + #.162 RO2-N. + #1.015 R2O2. + #.743 RCO-O2. + #.259 HCHO + #.234 CCHO + #.095 RCHO + #.509 ACET + #1.259 XC
		PF=KETONE QY = 2.0e-2			DIPK + HV = #.96 RO2-R. + #.04 RO2-N. + RCO-O2. + #.96 ACET + #.88 XC
Di-Isopropyl Ketone [AP]	5.38e-12	5.38e-12			DIPK + HO. = #.095 RO2-R. + #.162 RO2-N. + #1.015 R2O2. + #.743 RCO-O2. + #.259 HCHO + #.234 CCHO + #.509 ACET + #1.259 XC + #.095 PRD1
		PF=KETONE QY = 2.0e-2			DIPK + HV = #.96 RO2-R. + #.04 RO2-N. + RCO-O2. + #.96 ACET + #.88 XC
	6.47e-11	6.47e-11			PRD1 + HO. = #.004 RO2-R. + #.009 RO2-N. + #.055 R2O2. + #.988 RCO-O2. + #.01 HCHO + #.009 CCHO + #.004 RCHO + #.02 ACET + #.015 MGLY + #-0.16 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #.902 RO2-R. + #.098 RO2-N. + #.902 RCO-O2. + CO + #.902 CCHO + #-3.098 XC
2-Octanone [LP]	1.10e-11	1.10e-11			C8-KET-2 + HO. = #.515 RO2-R. + #.296 RO2-N. + #.914 R2O2. + #.18 CCO-O2. + #.009 RCO-O2. + #.014 HCHO + #.225 RCHO + #.487 PROD2 + #2.227 XC
		PF=KETONE QY = 1.0e-2			C8-KET-2 + HV = #.814 RO2-R. + #.186 RO2-N. + #.902 R2O2. + CCO-O2. + #.814 RCHO + #2.443 XC
2-Octanone [AP]	1.10e-11	1.10e-11			C8-KET-2 + HO. = #.515 RO2-R. + #.296 RO2-N. + #.914 R2O2. + #.18 CCO-O2. + #.009 RCO-O2. + #.014 HCHO + #.005 RCHO + #2.227 XC + #.22 PRD1 + #.487 PRD2
		PF=KETONE QY = 1.0e-2			C8-KET-2 + HV = #.814 RO2-R. + #.186 RO2-N. + #.902 R2O2. + CCO-O2. + #2.443 XC + #.814 PRD3
	2.94e-11	2.94e-11			PRD1 + HO. = #.159 HO2. + #.119 RO2-R. + #.025 RO2-N. + #.066 R2O2. + #.698 RCO-O2. + #.011 CO + #.001 HCHO + #.009 CCHO + #.288 RCHO + #.015 MGLY + #-0.185 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.044 CCHO + #.874 RCHO + #-1.465 XC
	1.89e-11	1.89e-11			PRD2 + HO. = #.47 HO2. + #.34 RO2-R. + #.073 RO2-N. + #.011 R2O2. + #.042 CCO-O2. + #.074 RCO-O2. + #.044 HCHO + #.174 CCHO + #.39 RCHO + #.533 PROD2 + #.02 MGLY + #.432 XC
	3.32e-11	3.32e-11			PRD3 + HO. = #.278 HO2. + #.124 RO2-R. + #.013 RO2-N. + #.585 RCO-O2. + #.009 CO + #.017 CCHO + #.427 RCHO + #.013 MGLY + #-0.199 XC
	3.80e-15	3.80e-15			PRD3 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD3 + HV = #.065 HO2. + #1.809 RO2-R. + #.126 RO2-N. + CO + #.077 CCHO + #.874 RCHO + #-1.531 XC
2-Nonanone [LP]	1.22e-11	1.22e-11			C9-KET-2 + HO. = #.503 RO2-R. + #.357 RO2-N. + #.87 R2O2. + #.14 CCO-O2. + #.149 RCHO + #.494 PROD2 + #3.167 XC
2-Nonanone [AP]	1.22e-11	1.22e-11			C9-KET-2 + HO. = #.503 RO2-R. + #.357 RO2-N. + #.87 R2O2. + #.14 CCO-O2. + #3.167 XC + #.149 PRD1 + #.494 PRD2
	3.06e-11	3.06e-11			PRD1 + HO. = #.129 HO2. + #.158 RO2-R. + #.045 RO2-N. + #.087 R2O2. + #.668 RCO-O2. + #.007 CO + #.316 RCHO + #.015 MGLY + #-0.276 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
		PF=C2CHO			PRD1 + HV = #.098 HO2. + #1.717 RO2-R. + #.186 RO2-N. + CO + #.86 RCHO + #-1.694 XC
	2.22e-11	2.22e-11			PRD2 + HO. = #.492 HO2. + #.327 RO2-R. + #.085 RO2-N. + #.039 CCO-O2. + #.057 RCO-O2. + #.062 CCHO + #.482 RCHO + #.588 PROD2 + #.013 MGLY + #.105 XC
Di-isobutyl ketone (2,6-dimethyl-4-heptanone) [LP]	2.75e-11	2.75e-11			DIBK + HO. = #.019 RO2-R. + #.282 RO2-N. + #1.401 R2O2. + #.014 C-O2. + #.685 RCO-O2. + #.594 HCHO + #.005 CCHO + #.123 RCHO + #.626 ACET + #.026 PROD2 + #2.232 XC
Di-isobutyl ketone (2,6-dimethyl-4-heptanone) [AP]	2.75e-11	2.75e-11			DIBK + HO. = #.019 RO2-R. + #.282 RO2-N. + #1.401 R2O2. + #.014 C-O2. + #.685 RCO-O2. + #.594 HCHO + #.005 CCHO + #.626 ACET + #2.232 XC + #.123 PRD1 + #.026 PRD2
	2.60e-11	2.60e-11			PRD1 + HO. = #.082 RO2-R. + #.004 RO2-N. + #.011 R2O2. + #.914 RCO-O2. + #.078 CO + #.011 HCHO + #.011 CCHO + #.004 RCHO + #.067 ACET + #-0.09 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD1 + HV = HO2. + #.96 RO2-R. + #.04 RO2-N. + CO + #.96 ACET + #-1.12 XC
	9.35e-12	9.35e-12			PRD2 + HO. = #.02 RO2-R. + #.222 RO2-N. + #1.439 R2O2. + #.014 C-O2. + #.038 CCO-O2. + #.706 RCO-O2. + #.626 HCHO + #.006 CCHO + #.083 RCHO + #.628 ACET + #.028 MEK + #.066 MGLY + #-0.618 XC
		PF=KETONE QY = 1.0e-2			PRD2 + HV = #.473 RO2-R. + #.075 RO2-N. + #.625 R2O2. + #.5 CCO-O2. + #.951 RCO-O2. + #.625 HCHO + #.307 RCHO + #.167 ACET + #-0.351 XC
2-Decanone [LP]	1.32e-11	1.32e-11			C10-K-2 + HO. = #.52 RO2-R. + #.396 RO2-N. + #.806 R2O2. + #.083 CCO-O2. + #.087 RCHO + #.517 PROD2 + #4.094 XC
2-Decanone [AP]	1.32e-11	1.32e-11			C10-K-2 + HO. = #.52 RO2-R. + #.396 RO2-N. + #.806 R2O2. + #.083 CCO-O2. + #4.094 XC + #.517 PRD1 + #.087 PRD2
	2.44e-11	2.44e-11			PRD1 + HO. = #.35 HO2. + #.402 RO2-R. + #.124 RO2-N. + #.036 R2O2. + #.057 CCO-O2. + #.067 RCO-O2. + #.028 HCHO + #.02 CCHO + #.538 RCHO + #.53 PROD2 + #.009 MGLY + #.053 XC
	3.01e-11	3.01e-11			PRD2 + HO. = #.073 HO2. + #.176 RO2-R. + #.078 RO2-N. + #.146 R2O2. + #.673 RCO-O2. + #.007 CO + #.26 RCHO + #.014 MGLY + #-0.316 XC
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + #-0 XC + XN
		PF=C2CHO			PRD2 + HV = #.135 HO2. + #1.613 RO2-R. + #.252 RO2-N. + CO + #.769 RCHO + #-1.819 XC
Methylvinyl ketone [LP]	1.89e-11	4.14e-12	-0.90		MVK + HO. = #.288 RO2-R. + #.039 RO2-N. + #.672 R2O2. + #.672 CCO-O2. + #.288 HCHO + #.672 CCHO + #.288 MGLY + #-0.079 XC
	4.58e-18	7.51e-16	3.02		MVK + O3 = #.164 HO. + #.064 HO2. + #.05 RO2-R. + #.05 RCO-O2. + #.475 CO + #.124 CO2 + #.1 HCHO + #.95 MGLY + #.351 HCOOH + #-0.05 XC
	0.00e+00				MVK + NO3 = #.039 RO2-N. + #.961 R2O2. + #.961 CCO-O2. + #.961 RCHO + #-1.039 XC + XN
	2.11e-12	2.11e-12			MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC
		PF=ACROLEIN QY = 2.1e-3			MVK + HV = #.3 C-O2. + #.3 MA-RCO3. + #.7 CO + #.7 PROD2 + #-2.4 XC
Methylvinyl ketone [AP]	1.89e-11	4.14e-12	-0.90		MVK + HO. = #.288 RO2-R. + #.039 RO2-N. + #.672 R2O2. + #.672 CCO-O2. + #.288 HCHO + #.672 CCHO + #.288 MGLY + #-0.079 XC
	4.58e-18	7.51e-16	3.02		MVK + O3 = #.164 HO. + #.064 HO2. + #.05 RO2-R. + #.05 RCO-O2. + #.475 CO + #.124 CO2 + #.1 HCHO + #.95 MGLY + #.351 HCOOH + #-0.05 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	0.00e+00				MVK + NO3 = #.039 RO2-N. + #.961 R2O2. + #.961 CCO-O2. + #-1.039 XC + #.961 PRD1 + XN
	2.11e-12	2.11e-12			MVK + O3P = #.55 MEK + #.45 XC + #.45 PRD2
	PF=ACROLEIN QY = 2.1e-3				MVK + HV = #.3 C-O2. + #.3 MA-RCO3. + #.7 CO + #-2.4 XC + #.7 PRD3
	1.93e-11	1.93e-11			PRD1 + HO. = RCO-O2. + XN
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + #2 XN
		PF=C2CHO			PRD1 + HV = NO2 + HO2. + CO + HCHO + XC
	6.11e-11	6.11e-11			PRD2 + HO. = RCO-O2.
	3.80e-15	3.80e-15			PRD2 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD2 + HV = RO2-R. + CCO-O2. + CO + HCHO + #-1 XC
	2.60e-11	2.60e-11			PRD3 + HO. = #.984 RO2-R. + #.016 RO2-N. + #.984 HCHO + #.984 CCHO + #2.952 XC
	1.05e-17	1.05e-17			PRD3 + O3 = #.32 HO. + #.06 HO2. + #.26 C-O2. + #.51 CO + #.135 CO2 + #.5 HCHO + #.5 CCHO + #.185 HCOOH + #.17 CCO-OH + #3.07 XC
	9.74e-15	9.74e-15			PRD3 + NO3 = #.949 RO2-R. + #.051 RO2-N. + #5.693 XC + XN
	4.01e-12	4.01e-12			PRD3 + O3P = #.45 RCHO + #.55 MEK + #2.45 XC
Hydroxy Acetone	3.02e-12	3.02e-12			HOACET + HO. = #.756 HO2. + #.034 RO2-R. + #.177 CCO-O2. + #.034 RCO-O2. + #.211 HCHO + #.789 MGLY + #-0.034 XC
	PF=KETONE QY = 1.5e-1				HOACET + HV = HO2. + CCO-O2. + HCHO
Methoxy Acetone	6.77e-12	6.77e-12			MEOACET + HO. = #.148 RO2-R. + #.039 RO2-N. + #.812 R2O2. + #.798 CCO-O2. + #.014 RCO-O2. + #.028 HCHO + #.148 MEK + #.791 INERT + #.712 XC
	PF=KETONE QY = 1.0e-1				MEOACET + HV = RO2-R. + CCO-O2. + #.079 HCHO + #.961 INERT + #.961 XC
Diacetone Alcohol [LP]	1.49e-12	1.49e-12			DIACTALC + HO. = #.233 RO2-R. + #.086 RO2-N. + #.681 R2O2. + #.618 CCO-O2. + #.063 RCO-O2. + #.388 HCHO + #.5 RCHO + #.143 ACET + #.207 MEK + #.026 MGLY + #.834 XC
	PF=KETONE QY = 2.0e-2				DIACTALC + HV = #.93 RO2-R. + #.07 RO2-N. + CCO-O2. + #.93 HCHO + #.93 ACET + #-0.14 XC
Diacetone Alcohol [AP]	1.49e-12	1.49e-12			DIACTALC + HO. = #.233 RO2-R. + #.086 RO2-N. + #.681 R2O2. + #.618 CCO-O2. + #.063 RCO-O2. + #.388 HCHO + #.143 ACET + #.207 MEK + #.026 MGLY + #.834 XC + #.5 PRD1
	PF=KETONE QY = 2.0e-2				DIACTALC + HV = #.93 RO2-R. + #.07 RO2-N. + CCO-O2. + #.93 HCHO + #.93 ACET + #-0.14 XC
	1.97e-11	1.97e-11			PRD1 + HO. = #.017 RO2-R. + #.001 RO2-N. + #.983 RCO-O2. + #.017 HCHO + #.017 MGLY + #-0.019 XC
	3.80e-15	3.80e-15			PRD1 + NO3 = RCO-O2. + XN
		PF=C2CHO			PRD1 + HV = #2 HO2. + CO + ACET + #-1 XC
Nitrobenzene [PM]	1.50e-13	1.50e-13	0.00	0.0	NO2-BENZ + HO. = #.236 HO2. + #.764 RO2-R. + #.207 GLY + #.236 PHEN + #.764 DCB1 + #1.114 XC
Para Toluene Isocyanate [PM]	5.90e-12	5.90e-12	0.00	0.0	P-TI + HO. = #.2 HO. + #.7 HO2. + #.15 MGLY + CRES
Toluene Diiso-cyanate [PM]	7.40e-12	7.40e-12	0.00	0.0	TDI + HO. = #.5 HO. + CRES
Methylene Diphenylene Diisocyanate [PM]	1.18e-11	1.18e-11	0.00	0.0	MDI + HO. = #.2 HO. + #.7 HO2. + #.15 MGLY + CRES
Dimethyl Amine [PM]	6.62e-11	2.89e-11	-0.49	0.0	DM-AMINE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Ethyl Amine [PM]	2.77e-11	1.47e-11	-0.38	0.0	ET-AMINE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Trimethyl Amine [PM]	6.11e-11	2.62e-11	-0.50	0.0	TM-AMINE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
Ethanolamine [PM]	3.15e-11	3.15e-11	0.00	0.0	ETOH-NH2 + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Dimethylaminoethanol [PM]	9.00e-11	9.00e-11	0.00	0.0	DMAE + HO. = #.96 RO2-R. + #.04 RO2-N. + #.5 HCHO + #.5 RCHO
Diethanol Amine [PM]	9.37e-11	9.37e-11	0.00	0.0	ETOH2-NH + HO. = #.96 RO2-R. + #.04 RO2-N. + #.5 HCHO + #.5 RCHO
Triethanolamine [PM]	1.16e-10	1.16e-10	0.00	0.0	ETOH3-N + HO. = #.905 RO2-R. + #.095 RO2-N. + #.5 HCHO + #.5 RCHO
N-Methyl-2-Pyrrolidone [PM]	2.15e-11	2.15e-11	0.00	0.0	NMP + HO. = #.92 HO2. + #.08 RO2-N. + #.46 RCHO + #.46 PROD2 + #.38 XC + XN
	1.26e-13	1.26e-13	0.00	0.0	NMP + NO3 = #.92 HO2. + #.08 RO2-N. + #.92 PROD2 + #-1 XC + XN
Methyl Chloride [PM]	4.36e-14	3.15e-13	1.16	2.0	CH3-CL + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Vinyl Chloride [PM]	6.97e-12	1.69e-12	-0.84	0.0	CL-ETHE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Ethyl Chloride [PM]	4.11e-13	6.94e-13	0.30	2.0	C2-CL + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Dichloro-methane [PM]	1.42e-13	7.69e-13	0.99	2.0	CL2-ME + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Methyl Bromide [PM]	4.02e-14	2.34e-13	1.04	2.0	ME-BR + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
1,1-Dichloroethane [PM]	2.60e-13	2.60e-13	0.00	0.0	11CL2-C2 + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
1,2-Dichloroethane [PM]	2.48e-13	9.90e-13	0.81	2.0	12CL2-C2 + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Ethyl Bromide [PM]	2.99e-13	2.72e-11	2.67	0.0	C2-BR + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Chloroform [PM]	1.03e-13	5.67e-13	1.00	2.0	CHCL3 + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
n-Propyl Bromide [PM]	1.18e-12	1.18e-12	0.00	0.0	C3-BR + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
1,1,1-Trichloroethane [PM]	1.19e-14	5.33e-13	2.24	2.0	111-TCE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
1,1,2-Trichloroethane [PM]	1.97e-13	4.00e-13	0.41	2.0	112CL3C2 + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
n-Butyl Bromide [PM]	2.46e-12	2.46e-12	0.00	0.0	C4-BR + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
1,2-Dibromoethane [PM]	2.22e-13	9.27e-13	0.84	2.0	11BR2-C2 + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Trans-1,2-Dichloroethene [PM]	2.34e-12	1.01e-12	-0.50	0.0	T-12-DCE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
2-(Cl-methyl)-3-Cl-Propene	3.16e-11	3.16e-11			CL2IBUTE + HO. = #.48 RO2-R. + #.039 RO2-N. + #.961 R2O2. + #.48 Cl. + #.961 HCHO + #.961 MEK + #-1.039 XC
	3.90e-19	3.90e-19			CL2IBUTE + O3 = #.707 HO. + #.04 RO2-R. + #.627 R2O2. + #.667 Cl. + #.167 CO + #.043 CO2 + #.667 HCHO + #.333 MEK + #.667 MGLY + #.123 HCOOH + #-0.333 XC
	1.00e-15	1.00e-15			CL2IBUTE + NO3 = #.039 RO2-N. + #1.921 R2O2. + #.961 Cl. + #.961 HCHO + #2.803 XC + XN

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
	5.60e-12	5.60e-12			CL2IBUTE + O3P = #.4 RCHO + #.6 MEK + #.4 XC
2-(Cl-methyl)-3-Cl-Propene [PM]	3.16e-11	3.16e-11	0.00	0.0	CL2IBUTE + HO. = #.481 HO2. + #.481 RO2-R. + #.039 RO2-N. + #.961 R2O2. + #.961 HCHO + #.961 MEK + #-1.039 XC
	3.90e-19	3.90e-19	0.00	0.0	CL2IBUTE + O3 = #.707 HO. + #.667 HO2. + #.04 RO2-R. + #.627 R2O2. + #.167 CO + #.043 CO2 + #.667 HCHO + #.333 MEK + #.667 MGLY + #.123 HCOOH + #-0.333 XC
	1.00e-15	1.00e-15	0.00	0.0	CL2IBUTE + NO3 = #.961 HO2. + #.039 RO2-N. + #1.923 R2O2. + #.961 HCHO + #2.807 XC + XN
	5.60e-12	5.60e-12	0.00	0.0	CL2IBUTE + O3P = #.4 RCHO + #.6 MEK + #.4 XC
Trichloroethylene [PM]	2.36e-12	5.63e-13	-0.85	0.0	CL3-ETHE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Perchloro-ethylene [PM]	1.67e-13	9.64e-12	2.40	0.0	CL4-ETHE + HO. = RO2-R. + #.5 HCHO + #.5 RCHO
Monochloro-benzene [PM]	7.70e-13	7.70e-13	0.00	0.0	CL-BEN + HO. = #.236 HO2. + #.764 RO2-R. + #.207 GLY + #.236 PHEN + #.764 DCB1 + #1.114 XC
Benzotrifluoride [PM]	4.60e-13	4.60e-13	0.00	0.0	CF3-BEN + HO. = #.234 HO2. + #.758 RO2-R. + #.008 RO2-N. + #.116 GLY + #.135 MGLY + #.234 CRES + #.085 BALD + #.46 DCB1 + #.156 DCB2 + #.057 DCB3 + #1.178 XC
p-Dichloro-benzene [PM]	5.55e-13	5.55e-13	0.00	0.0	CL2-BEN + HO. = #.236 HO2. + #.764 RO2-R. + #.207 GLY + #.236 PHEN + #.764 DCB1 + #1.114 XC
p-Trifluoromethyl-Cl-Benzene [PM]	2.40e-13	2.40e-13	0.00	0.0	PCBTF + HO. = #.234 HO2. + #.758 RO2-R. + #.008 RO2-N. + #.116 GLY + #.135 MGLY + #.234 CRES + #.085 BALD + #.46 DCB1 + #.156 DCB2 + #.057 DCB3 + #1.178 XC
Isoprene Product #1	7.00e-11	7.00e-11			IP-MHY1 + HO. = #.701 RO2-R. + #.049 RO2-N. + #.25 MA-RCO3. + #.425 CO + #.276 CCHO + #.425 PROD2 + #.276 MGLY + #-0.649 XC
	1.00e-17	1.00e-17			IP-MHY1 + O3 = #.202 HO. + #.002 HO2. + #.1 RO2-R. + #.1 RCO-O2. + #.102 CO + #.202 HCHO + #.1 CCHO + #.9 MGLY + #.798 RCO-OH + #-0.898 XC
	1.00e-13	1.00e-13			IP-MHY1 + NO3 = #.935 RO2-R. + #.065 RO2-N. + #.935 CO + #.935 RNO3 + #-1.935 XC + #.065 XN
	2.47e-11	2.47e-11			IP-MHY1 + O3P = RCHO + #2 XC
	PF=ACROLEIN QY = 4.1e-3				IP-MHY1 + HV = HO2. + CCO-O2. + CO + CCHO
Isoprene Product #2	7.00e-11	7.00e-11			IP-MHY2 + HO. = #.701 RO2-R. + #.049 RO2-N. + #.25 MA-RCO3. + #.425 CO + #.276 CCHO + #.425 PROD2 + #.276 MGLY + #-0.649 XC
	1.00e-17	1.00e-17			IP-MHY2 + O3 = #.202 HO. + #.002 HO2. + #.1 RO2-R. + #.1 RCO-O2. + #.102 CO + #.202 HCHO + #.1 CCHO + #.9 MGLY + #.798 RCO-OH + #-0.898 XC
	1.00e-13	1.00e-13			IP-MHY2 + NO3 = #.935 RO2-R. + #.065 RO2-N. + #.935 CO + #.935 RNO3 + #-1.935 XC + #.065 XN
	2.47e-11	2.47e-11			IP-MHY2 + O3P = RCHO + #2 XC
	PF=ACROLEIN QY = 4.1e-3				IP-MHY2 + HV = HO2. + CCO-O2. + CO + CCHO
Isoprene Product #3	7.00e-11	7.00e-11			IP-HMY + HO. = #.701 RO2-R. + #.049 RO2-N. + #.25 MA-RCO3. + #.016 CO + #.042 HCHO + #.057 RCHO + #.644 MEK + #.644 GLY + #-0.385 XC
	1.00e-17	1.00e-17			IP-HMY + O3 = #.55 HO. + #1.442 HO2. + #.004 RO2-R. + #.004 RCO-O2. + #1.35 CO + #.45 CO2 + #.004 HCHO + #.9 MEK + #.1 GLY + #.096 MGLY + #-0.904 XC
	1.00e-13	1.00e-13			IP-HMY + NO3 = #.935 RO2-R. + #.065 RO2-N. + #.935 HCHO + #.935 RCHO + #.87 XC + XN
	2.47e-11	2.47e-11			IP-HMY + O3P = #.6 RCHO + #.4 MGLY + #2 XC
	PF=ACROLEIN QY = 4.1e-3				IP-HMY + HV = #2 HO2. + #2 CO + MEK + #-1 XC

Table A-6 (continued)

Compound [a]	Rate Parameters [b] k(298)	A	Ea	B	Reactions and Products [c]
PROD2 Species #1	9.63e-12	9.63e-12			PROD2-1 + HO. = #.34 HO2. + #.529 RO2-R. + #.037 RO2-N. + #.084 CCO-O2. + #.01 RCO-O2. + #.444 HCHO + #.953 RCHO + #1.277 XC
	PF=KETONE QY = 5.0e-2				PROD2-1 + HV = RO2-R. + #.013 R2O2. + CCO-O2. + #.033 HCHO + #.002 CCHO + #.987 RCHO + #-0 XC
PROD2 Species #2	1.45e-11	1.45e-11			PROD2-2 + HO. = #.201 HO2. + #.666 RO2-R. + #.071 RO2-N. + #.062 CCO-O2. + #.612 HCHO + #.007 CCHO + #.345 RCHO + #.577 MEK + #1.483 XC
	PF=KETONE QY = 2.0e-2				PROD2-2 + HV = #.949 RO2-R. + #.051 RO2-N. + #.748 R2O2. + CCO-O2. + #1.484 HCHO + #.736 CCHO + #.213 RCHO + #.1 XC
PROD2 Species #3	1.52e-11	1.52e-11			PROD2-3 + HO. = #.451 HO2. + #.393 RO2-R. + #.061 RO2-N. + #.094 RCO-O2. + #.008 HCHO + #.3 CCHO + #.347 RCHO + #.551 PROD2 + #1.396 XC
	PF=KETONE QY = 1.0e-2				PROD2-3 + HV = #.93 RO2-R. + #.07 RO2-N. + #.785 R2O2. + RCO-O2. + #.93 RCHO + #.789 XC
PROD2 Species #4	1.83e-11	1.83e-11			PROD2-4 + HO. = #.491 HO2. + #.359 RO2-R. + #.075 RO2-N. + #.075 RCO-O2. + #.086 CCHO + #.53 RCHO + #.568 PROD2 + #2.153 XC
PROD2 Species #5	1.97e-11	1.97e-11			PROD2-5 + HO. = #.41 HO2. + #.415 RO2-R. + #.108 RO2-N. + #.066 RCO-O2. + #.029 CCHO + #.614 RCHO + #.527 PROD2 + #3.089 XC
RNO3 Species #1	1.60e-12	1.60e-12			RNO3-1 + HO. = #.572 NO2 + #.354 RO2-R. + #.074 RO2-N. + #.684 R2O2. + #1.022 CCHO + #.199 RCHO + #.061 MEK + #.156 RNO3 + #-0.259 XC + #.272 XN
		PF=IC3ONO2			RNO3-1 + HV = NO2 + #.606 HO2. + #.394 RO2-R. + #.789 CCHO + #.606 MEK
RNO3 Species #2	1.15e-11	1.15e-11			RNO3-2 + HO. = #.008 NO2 + #.611 HO2. + #.357 RO2-R. + #.024 RO2-N. + #.007 HCHO + #.124 CCHO + #.145 RCHO + #.831 RNO3 + #-0.82 XC + #.161 XN
		PF=IC3ONO2			RNO3-2 + HV = NO2 + HO2. + PROD2 + #-1 XC
RNO3 Species #3	4.70e-12	4.70e-12			RNO3-3 + HO. = #.731 NO2 + #.134 RO2-R. + #.135 RO2-N. + #1.029 R2O2. + #.012 HCHO + #1.08 CCHO + #.071 RCHO + #.544 MEK + #.03 PROD2 + #.07 RNO3 + #.022 XC + #.198 XN
		PF=IC3ONO2			RNO3-3 + HV = NO2 + #.919 RO2-R. + #.081 RO2-N. + #.307 R2O2. + #1.535 CCHO + #.495 MEK + #.101 PROD2 + #-0.143 XC
RNO3 Species #4	9.89e-12	9.89e-12			RNO3-4 + HO. = #.103 NO2 + #.065 HO2. + #.72 RO2-R. + #.111 RO2-N. + #.006 CCHO + #.576 RCHO + #.102 PROD2 + #.217 RNO3 + #2.679 XC + #.679 XN
		PF=IC3ONO2			RNO3-4 + HV = NO2 + #.441 HO2. + #.483 RO2-R. + #.075 RO2-N. + #.441 HCHO + #.441 RCHO + #.483 PROD2 + #1.882 XC
RNO3 Species #5	5.64e-12	5.64e-12			RNO3-5 + HO. = #.597 NO2 + #.125 RO2-R. + #.277 RO2-N. + #1.108 R2O2. + #.041 HCHO + #.401 CCHO + #.268 RCHO + #.035 ACET + #.454 MEK + #.143 PROD2 + #.039 RNO3 + #1.674 XC + #.364 XN
		PF=IC3ONO2			RNO3-5 + HV = NO2 + #.826 RO2-R. + #.174 RO2-N. + #.563 R2O2. + #.362 HCHO + #.261 CCHO + #.439 RCHO + #.119 ACET + #.358 MEK + #.268 PROD2 + #1.361 XC
RNO3 Species #6	9.87e-12	9.87e-12			RNO3-6 + HO. = #.018 NO2 + #.563 RO2-R. + #.419 RO2-N. + #.755 R2O2. + #.001 CCHO + #.021 RCHO + #.015 PROD2 + #.546 RNO3 + #4.052 XC + #.436 XN
		PF=IC3ONO2			RNO3-6 + HV = NO2 + #.76 RO2-R. + #.24 RO2-N. + #.042 R2O2. + #.76 PROD2 + #4 XC

[a] If the code [PM] follows the species name, then parameterized mechanism was employed (see Section IV). Otherwise, the mechanism was produced using the mechanism generation system as discussed in Section III. For some VOCs whose mechanisms were produced by the mechanism generation system, separate mechanisms

Table A-6 (continued)

are given depending on how the major reactive organic photooxidation products are represented. If the code [AP] follows the compound name, separate reactions are included to explicitly represent the major reactive products, using the added model species PRD1, PRD2,…, whose mechanisms were using the mechanism generation system to represent the specific products formed from these compounds. This mechanism is used in model simulations of the atmospheric reactivities of the compound, but not when representing the compound when present in mixtures. If the code [LP] follows the compound name, or if no code is given, then the standard set of lumped model species were used to represent all the reactive products.

[b] See footnotes to Table A-2.