

*Appendix I*COMPOUNDS AND REACTIONS IN THE EXPLICIT
ISOPRENE MECHANISM

functional group	abbreviation
carbonyl	CO
nitrate	N
hydroxy	OH
hydroperoxy	OOH
epoxide	##O ^a
alkyl radical	R
alkoxy radical	O
peroxy radical	OO
double bond	## ^b

Table I.1: Abbreviations for functional groups used in the naming of compounds in the explicit isoprene mechanism. ^a## are the two carbon numbers the epoxide is attached to; ^b## are the two carbon numbers the double bond is attached to.

Table I.2: Names used for compounds in the explicit isoprene mechanism. Italics denote radical species; bold font denotes species with no further chemistry in the model.

common / IUPAC name	our name	MCM name
Isoprene	ISOP	C5H8
<i>cis</i> -OH-isoprene-adduct 1 addition	<i>ISOP1OHc</i>	CISOPA
<i>trans</i> -OH-isoprene-adduct 1 addition	<i>ISOP1OHt</i>	TISOPA
<i>cis</i> -OH-isoprene-adduct 4 addition	<i>ISOP4OHc</i>	CISOPC
<i>trans</i> -OH-isoprene-adduct 1 addition	<i>ISOP4OHt</i>	TISOPC
<i>E</i> -(4,1)-ISOP00	<i>ISOP1004OHt</i>	ISOPCO2
<i>Z</i> -(4,1)-ISOP00	<i>ISOP1004OHc</i>	CISOPCO2
<i>Z</i> -(1,4)-ISOP00	<i>ISOP10H400c</i>	CISOPAO2
<i>E</i> -(1,4)-ISOP00	<i>ISOP10H400t</i>	ISOPAO2
(1,2)-ISOP00	<i>ISOP10H200</i>	<i>ISOPB02</i>
(4,3)-ISOP00	<i>ISOP30040H</i>	<i>ISOPD02</i>
peroxy radical from ISOP10H400 + NO (major)	<i>ISOP1CO200300H40H</i>	C52602
peroxy radical from ISOP10H400 + NO (minor)	<i>ISOP1CO200H30040H</i>	-
peroxy radical from ISOP10H400 + NO (major)	<i>ISOP1OH200300H4CO</i>	-
peroxy radical from ISOP10040H + NO (minor)	<i>ISOP1OH200H3004CO</i>	C52702
RO₂ + RO₂ PRODUCTS		
(1,2)-isoprene diol	ISOP10H20H	ISOPBOH
(3,4)-isoprene diol	ISOP30H40H	ISOPDOH
(1,4)-isoprene diol	ISOP10H40H	ISOPA0H
1-hydroxy-3-methylbut-3-en-2-one	ISOP3CO40H	HCOC5
4-hydroxy-2-methylbut-2-en-1-al	ISOP1CO40H	HC4CCHO
4-hydroxy-3-methylbut-2-en-1-al	ISOP10H4CO	HC4ACHO
peroxy radical from ISOP3CO40H	<i>ISOP1OH2003CO40H</i>	C5902
3-hydroperoxy-1,4-dihydroxy-3-methylbutan-2-one	ISOP10H200H3CO40H	C5900H
1,4-dihydroxy-3-methyl-3-nitroxybutan-2-one	ISOP10H2N3CO40H	-
ISOPOOH		
(1,2)-ISOPOOH	ISOP10H200H	ISOPBOOH

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<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	(4,3)-ISOPOOH	ISOP3OOH4OH	ISOPDOOH
	(1,4)-ISOPOOH	ISOP1OOH4OH	ISOPCOOH
	(4,1)-ISOPOOH	ISOP1OH4OOH	ISOPA00H
	alkoxy radical from (1,2)-ISOPOOH + OH	<i>ISOP1OH2OOH3R4OH</i>	-
	alkoxy radical from (4,3)-ISOPOOH + OH	<i>ISOP1OH2R3OOH4OH</i>	-
	peroxy radical from (1,2)-ISOPOOH + OH (major)	<i>ISOP1OH2OOH3OO4OH</i>	-
	peroxy radical from (1,2)-ISOPOOH + OH (minor)	<i>ISOP1OH2OOH3OH4OO</i>	-
	peroxy radical from (1,2)-ISOPOOH + OH (minor)	<i>ISOP1OH2OO3OH4OOH</i>	-
	peroxy radical from (4,3)-ISOPOOH + OH (major)	<i>ISOP1OH2OO3OOH4OH</i>	-
	peroxy radical from (4,3)-ISOPOOH + OH (minor)	<i>ISOP1OO2OH3OOH4OH</i>	-
	peroxy radical from (4,3)-ISOPOOH + OH (minor)	<i>ISOP1OOH2OH3OO4OH</i>	-
	isoprene 2,4-diperoxy-1,3-diol; ISOP(OOH) ₂	ISOP1OH2OOH3OH4OOH	-
	isoprene 1,3-diperoxy-2,4-diol; ISOP(OOH) ₂	ISOP1OOH2OH3OOH4OH	-
	isoprene 2,3-diperoxy-1,4-diol; ISOP(OOH) ₂	ISOP1OH2OOH3OOH4OH	-
	3-hydroperoxy-2,4-hydroxy-3-methylbutanal	ISOP1OH2OOH3OH4CO	C580OH
	2-hydroperoxy-3-methyl-4-nitrooxybutane-1,3-diol	ISOPIN2OH3OOH4OH	INCOOH
	2-hydroperoxy-2-methyl-4-nitrooxybutane-1,3-diol	ISOP1OH2OOH3OH4N	INAOOH
	4-hydroperoxy-2-methyl-2-nitrooxybutane-1,3-diol	ISOP1OH2N3OH4OOH	INB2OOH
	4-hydroperoxy-3-methyl-2-nitrooxybutane-1,3-diol	ISOP1OOH2OH3N4OH	-
	2-hydroperoxy-2-methyl-3-nitrooxybutane-1,4-diol	ISOP1OH2OOH3N4OH	INDOOH
	3-hydroperoxy-2-methyl-2-nitrooxybutane-1,4-diol	ISOP1OH2N3OOH4OH	INB1OOH
	IEPOX AND OTHER EPOXIDES		
	<i>trans</i> - β -IEPOX	ISOP1OH23O4OHt	IEPOXB
	<i>cis</i> - β -IEPOX	ISOP1OH23O4OHc	IEPOXB
	δ 1-IEPOX	ISOP1OH2OH34O	IEPOXA
	δ 4-IEPOX	ISOP12O3OH4OH	IEPOXC
	1,2-epoxy-3-hydroperoxy-2-methylbutane-1,4-diol	ISOP1OH12O3OOH4OH	-
	1,2-epoxy-3-hydroperoxy-3-methylbutane-1,4-diol	ISOP1OH2OOH34O4OH	-
	2,3-epoxy-3-methyl-4-nitrooxybutan-1-ol	ISOPIN23O4OH	-
	2,3-epoxy-2-methyl-4-nitrooxybutan-1-ol	ISOP1OH23O4N	-
	3,4-epoxy-2-methyl-1-nitrooxybutan-2-ol	ISOPIN2OH34O	-
	3,4-epoxy-3-methyl-1-nitrooxybutan-2-ol	ISOP12O3OH4N	-
	3,4-epoxy-1-hydroperoxy-3-methylbutan-2-ol	ISOP12O3OH4OOH	-
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common / IUPAC name	our name	MCM name
3,4-epoxy-1-hydroperoxy-2-methylbutan-2-ol	ISOP100H20H34O	-
2,3-epoxy-4-hydroxy-3-methylbutanal	ISOP10H23O4CO	IEB4CHO
2,3-epoxy-4-hydroxy-2-methylbutanal	ISOP1CO23O4OH	IEB1CHO
3,4-epoxy-2-hydroxy-3-methylbutanal	ISOP12O30H4CO	IECCHO
3,4-epoxy-1-hydroxy-3-methylbutan-2-one	ISOP12O3CO4OH	-
3,4-epoxy-2-hydroxy-2-methylbutanal	ISOP1CO20H34O	IEACHO
2,3-epoxy-3-methyl-4-nitroxybutanal	ISOPIN23O4CO	-
2,3-epoxy-2-methyl-4-nitroxybutanal	ISOP1CO23O4N	-
1,2-epoxy-2-methylbut-3-en-1-ol	ISOP1OH12O	-
3,4-epoxy-2-methylbut-1-en-1-al	ISOP121CO34O	-
3,4-epoxy-3-methylbut-1-en-1-al	ISOP12O344CO	-
alkyl radical from <i>cis</i> - β -IEPOX (major)	<i>ISOP1OH1R23O4OHc</i>	-
alkyl radical from <i>cis</i> - β -IEPOX (minor)	<i>ISOP1OH23O4R4OHc</i>	-
alkyl radical from <i>trans</i> - β -IEPOX (major)	<i>ISOP1OH1R23O4OHt</i>	-
alkyl radical from <i>trans</i> - β -IEPOX (minor)	<i>ISOP1OH23O4R4OHt</i>	-
alkyl radical from δ 4-IEPOX	<i>ISOP12O30H3R4OH</i>	-
alkyl radical from β -INHE (major)	<i>ISOP1OH1R23O4N</i>	-
alkyl radical from β -INHE (minor)	<i>ISOPIN23O4OH4R</i>	-
alkyl radical from δ 4-INHE	<i>ISOP12O30H3R4N</i>	-
2,4-dihydroxy-3-methylbutanal	ISOP1OH3OH4CO	-
ISOPOO ISOMERIZATION AND HPALD		
HPALD1 (from Z-(1,4)-ISOPOO)	ISOP1CO400Hc	C5HPALD1
HPALD2 (from Z-(4,1)-ISOPOO)	ISOP100H4COc	C5HPALD2
HPALD from (1,2)-ISOPOOH	ISOP1CO200H	-
HPALD from (4,3)-ISOPOOH	ISOP300H4CO	-
alkyl radical from HPALD1 + OH addition	<i>ISOP1CO20H3R40OH</i>	-
alkyl radical from HPALD1 + OH abstraction	<i>ISOP1CO3R40OH</i>	-
alkyl radical from HPALD2 + OH addition	<i>ISOP100H2R3OH4CO</i>	-
alkyl radical from HPALD2 + OH abstraction	<i>ISOP100H2R4CO</i>	-
peroxy radical from HPALD1 + OH abstraction	<i>ISOP1CO400c</i>	-
peroxy radical from HPALD1 + OH abstraction	<i>ISOP1CO200</i>	-
peroxy radical from HPALD1 + OH addition (major)	<i>ISOP1CO2003OH40OH</i>	-
peroxy radical from HPALD1 + OH addition (minor)	<i>ISOP1CO20H30040OH</i>	-

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<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	peroxy radical from HPALD2 + OH abstraction	<i>ISOP1004COc</i>	-
	peroxy radical from HPALD2 + OH abstraction	<i>ISOP3004CO</i>	-
	peroxy radical from HPALD2 + OH addition (major)	<i>ISOP100H20030H4CO -</i>	HPC52O2
	peroxy radical from HPALD2 + OH addition (minor)	<i>ISOP100H200H3004CO</i>	-
	peroxy radical from 1,6 H-shift of ISOP10H400c	<i>ISOP1CO200300H400H</i>	C536O2
	peroxy radical from 1,6 H-shift of ISOP10H400c	<i>ISOP1CO200H300400H</i>	-
	peroxy radical from 1,6 H-shift of ISOP10H400c	<i>ISOP1CO200H300H400</i>	-
	peroxy radical from 1,6 H-shift of ISOP10040Hc	<i>ISOP100H200H3004CO</i>	C537O2
	peroxy radical from 1,6 H-shift of ISOP10040Hc	<i>ISOP100H200300H4CO</i>	-
	peroxy radical from 1,6 H-shift of ISOP10040Hc	<i>ISOP100200H300H4CO</i>	-
	C ₅ peroxy acid aldehyde (PACALD) from HPALD1	ISOP1CO100H4CO	C5PACALD1
	C ₅ peroxy acid aldehyde (PACALD) from HPALD2	ISOP1CO4CO400H	C5PACALD2
	C ₅ ketene peroxy radical from HPALD1	<i>ISOP121CO300400H</i>	-
	C ₅ ketene peroxy radical from HPALD2	<i>ISOP100H200344CO</i>	-
	C ₄ hydroxy vinyl peroxy radical from HPALD1	C4HVP1	-
	C ₄ hydroxy vinyl peroxy radical from HPALD2	C4HVP2	-
	2-methylbut-2-ene-1,4-dial	ISOP1CO4CO	C4MDIAL
	3,4-dihydroperoxy-2-methyl-2-nitrooxybutanal	ISOP1CO2N300H400H	-
	2,4-dihydroperoxy-2-methyl-3-nitrooxybutanal	ISOP1CO200H3N400H	-
	2,3-dihydroperoxy-2-methyl-4-nitrooxybutanal	ISOP1CO200H300H4N	-
	3,4-dihydroperoxy-3-methyl-2-nitrooxybutanal	ISOP100H200H3N4CO	-
	2,4-dihydroperoxy-3-methyl-3-nitrooxybutanal	ISOP100H2N300H4CO	-
	2,3-dihydroperoxy-3-methyl-4-nitrooxybutanal	ISOP1N200H300H4CO	-
	2,3,4-trihydroperoxy-2-methylbutanal	ISOP1CO200H300H400H	C53600H
	2,3,4-trihydroperoxy-3-methylbutanal	ISOP100H200H300H4CO	C53700H
	DAYTIME NITRATES		
	(1,2) β isoprene hydroxy nitrate (IHN)	ISOP1OH2N	ISOPBNO3
	(4,3) β isoprene hydroxy nitrate (IHN)	ISOP3N4OH	ISOPDNO3
	Z- δ (1,4) isoprene hydroxy nitrate (IHN)	ISOP1OH4Nc	ISOPANO3
	E- δ (1,4) isoprene hydroxy nitrate (IHN)	ISOP1OH4Nt	ISOPANO3
	Z- δ (4,1) isoprene hydroxy nitrate (IHN)	ISOP1N4OHc	ISOPCNO3
	E- δ (4,1) isoprene hydroxy nitrate (IHN)	ISOP1N4Oht	ISOPCNO3
	alkyl radical from (1,2)-IHN + OH	<i>ISOP1OH2N3R4OH</i>	-

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<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	alkyl radical from (4,3)-IHN + OH	<i>ISOP1OH2R3N4OH</i>	-
	peroxy radical from (1,2)-IHN + OH	<i>ISOP1OH2N3OO4OH</i>	INB1O2
	peroxy radical from (1,2)-IHN + OH	<i>ISOP1OH2N3OH4OO</i>	INB2O2
	peroxy radical from (4,3)-IHN + OH	<i>ISOP1OH2OO3N4OH</i>	INDO2
	peroxy radical from (4,3)-IHN + OH	<i>ISOP1OO2OH3N4OH</i>	-
	3-hydroperoxy-4-hydroxy-3-methyl-2-nitrooxybutanal	ISOP1OH2OOH3N4CO	C527NO3
	3-hydroperoxy-4-hydroxy-2-methyl-2-nitrooxybutanal	ISOP1CO2N3OOH4OH	C526NO3
	2-hydroperoxy-4-hydroxy-2-methyl-3-nitrooxybutanal	ISOP1CO2OOH3N4OH	INDHPCHO
	2-hydroperoxy-4-hydroxy-3-methyl-3-nitrooxybutanal	ISOP1OH2N3OOH4CO	INB1HPCHO
	4-hydroperoxy-3-hydroxy-2-methyl-2-nitrooxybutanal	ISOP1CO2N3OH4OOH	-
	4-hydroperoxy-3-hydroxy-3-methyl-2-nitrooxybutanal	ISOP1OOH2OH3N4CO	-
	2-methyl-2,3-dinitrooxybutane-1,4-diol	ISOP1OH2N3N4OH	INB1NO3
	2-methyl-2,4-dinitrooxybutane-1,3-diol	ISOP1OH2N3OH4N	INANO3
	3-methyl-2,4-dinitrooxybutane-1,3-diol	ISOP1N2OH3N4OH	INCNO3
	2,3-dihydroperoxy-4-hydroxy-2-methylbutanal	ISOP1CO2OOH3OOH4OH	C526OOH
	2,3-dihydroperoxy-4-hydroxy-3-methylbutanal	ISOP1OH2OOH3OOH4CO	C527OOH
	NIGHTTIME NITRATES		
	peroxy radical from isoprene + NO ₃	<i>ISOP1N2OO</i>	-
	peroxy radical from isoprene + NO ₃	<i>ISOP1N4OO</i>	NISOP02
	peroxy radical from isoprene + NO ₃	<i>ISOP3OO4N</i>	-
	peroxy radical from isoprene + NO ₃	<i>ISOP1OO4N</i>	-
	alkoxy radical from ISOP1N4OO	<i>ISOP1N4O</i>	NISOP0
	alkoxy radical from ISOP1OO4N	<i>ISOP1O4N</i>	-
	(2,1) isoprene hydroperoxy nitrate (IPN)	ISOP1N2OOH	-
	(4,1) isoprene hydroperoxy nitrate (IPN)	ISOP1N4OOH	-
	(3,4) isoprene hydroperoxy nitrate (IPN)	ISOP3OOH4N	NISOP0OH
	(1,4) isoprene hydroperoxy nitrate (IPN)	ISOP1OOH4N	-
	(2,1) isoprene hydroxy nitrate (IHN)	ISOP1N2OH	-
	(3,4) isoprene hydroxy nitrate (IHN)	ISOP3OH4N	ISOP34NO3
	(4,1) isoprene carbonyl nitrate (ICN)	ISOP1N4CO	NC4CHO
	(1,4) isoprene carbonyl nitrate (ICN)	ISOP1CO4N	-
	(3,4) isoprene carbonyl nitrate (ICN)	ISOP3CO4N	-
	(1,2) isoprene dinitrate	ISOP1N2N	-

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<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	(1,4) isoprene dinitrate	ISOPIN4N	NISOPNO3
	(3,4) isoprene dinitrate	ISOP3N4N	-
	alkyl radical from (1,4)-IHN + OH	ISOP1OH2OH3R4N	-
	alkyl radical from (4,1)-IHN + OH	ISOP1N2R3OH4OH	-
	alkyl radical from (2,1)-IPN + OH	ISOP1N2OOH3R4OH	-
	alkyl radical from (4,1)-IPN + OH (major)	ISOP1N2OH3R4OOH	-
	alkyl radical from (4,1)-IPN + OH (minor)	ISOP1N2R3OH4OOH	-
	alkyl radical from (3,4)-IPN + OH	ISOP1OH2R3OOH4N	-
	alkyl radical from (1,4)-IPN + OH (major)	ISOP1OOH2R3OH4N	-
	alkyl radical from (1,4)-IPN + OH (minor)	ISOP1OOH2OH3R4N	-
	alkyl radical from (4,1)-ICN + OH	ISOP1N2R3OH4CO	-
	alkyl radical from (1,4)-ICN + OH	ISOP1CO2OH3R4N	-
	alkyl radical from (4,1)-ICN + OH	ISOP1N4R4CO	-
	alkyl radical from (1,4)-ICN + OH	ISOP1CO1R4N	-
	peroxy radical from (4,1)-IHN + OH (major)	ISOP1N2OO3OH4OH	-
	peroxy radical from (4,1)-IHN + OH (minor)	ISOP1N2OH3OO4OH	INCO2
	peroxy radical from (1,4)-IHN + OH (major)	ISOP1OH2OO3OH4N	INAO2
	peroxy radical from (1,4)-IHN + OH (minor)	ISOP1OH2OH3OO4N	-
	peroxy radical from (3,4)-IHN + OH	ISOP1OO2OH3OH4N	-
	peroxy radical from (2,1)-IHN + OH	ISOP1N2OH3OH4OO	-
	peroxy radical from (2,1)-IPN + OH (major)	ISOP1N2OO3OOH4OH	-
	peroxy radical from (2,1)-IPN + OH (minor)	ISOP1N2OOH3OO4OH	-
	peroxy radical from (2,1)-IPN + OH (minor)	ISOP1N2OOH3OH4OO	-
	peroxy radical from (4,1)-IPN + OH (major)	ISOP1N2OO3OH4OOH	-
	peroxy radical from (4,1)-IPN + OH (minor)	ISOP1N2OH3OO4OOH	-
	peroxy radical from (4,1)-IPN + OH (minor)	ISOP1N2OH3OOH4OO	-
	peroxy radical from (3,4)-IPN + OH (major)	ISOP1OH2OO3OOH4N	-
	peroxy radical from (3,4)-IPN + OH (minor)	ISOP1OH2OOH3OO4N	-
	peroxy radical from (3,4)-IPN + OH (minor)	ISOP1OH2OOH3OH4N	-
	peroxy radical from (1,4)-IPN + OH (major)	ISOP1OOH2OO3OH4N	-
	peroxy radical from (1,4)-IPN + OH (minor)	ISOP1OOH2OH3OO4N	-
	peroxy radical from (1,4)-IPN + OH (minor)	ISOP1OO2OOH3OH4N	-
	peroxy radical from (4,1)-ICN + OH (major)	ISOP1N2OO3OH4CO	C51002

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<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	peroxy radical from (4,1)-ICN + OH (minor)	<i>ISOP1N2OH3OO4CO</i>	-
	peroxy radical from (4,1)-ICN + OH (minor)	<i>ISOP1N2OO344CO</i>	-
	peroxy radical from (4,1)-ICN + OH (minor)	<i>ISOP1N4CO4OO</i>	NC4CO3
	peroxy radical from (1,4)-ICN + OH (major)	<i>ISOP1CO2OO3OH4N</i>	-
	peroxy radical from (1,4)-ICN + OH (minor)	<i>ISOP1CO2OH3OO4N</i>	-
	peroxy radical from (1,4)-ICN + OH (minor)	<i>ISOP121CO3OO4N</i>	-
	peroxy radical from (1,4)-ICN + OH (minor)	<i>ISOP1CO1OO4N</i>	-
	peroxy radical from (1,4)-INHE + OH	<i>ISOP1OH2OO3CO4N</i>	-
	peroxy radical from (4,1)-INHE + OH	<i>ISOP1N2OO3CO4OH</i>	-
	C ₄ nitrooxy vinyl peroxy radical from (1,4)-ICN	<i>C4NVP1</i>	-
	C ₄ nitrooxy vinyl peroxy radical from (4,1)-ICN	<i>C4NVP2</i>	-
	3-methyl-3,4-dinitrooxybutane-1,2-diol	ISOP1N2N3OH4OH	-
	2-methyl-3,4-dinitrooxybutane-1,2-diol	ISOP1OH2OH3N4N	-
	2-methyl-1,4-dinitrooxybutane-2,3-diol	ISOP1N2OH3OH4N	-
	3-hydroperoxy-3-methyl-4-nitrooxybutane-1,2-diol	ISOP1N2OOH3OH4OH	-
	4-hydroperoxy-2-methyl-4-nitrooxybutane-1,2-diol	ISOP1OH2OH3OOH4N	-
	4-hydroperoxy-2-methyl-1-nitrooxybutane-2,3-diol	ISOP1N2OH3OH4OOH	-
	1-hydroperoxy-2-methyl-4-nitrooxybutane-2,3-diol	ISOP1OOH2OH3OH4N	-
	3-hydroperoxy-3-methyl-2,4-dinitrooxybutan-1-ol	ISOP1N2OOH3N4OH	-
	3-hydroperoxy-3-methyl-1,4-dinitrooxybutan-2-ol	ISOP1N2OOH3OH4N	-
	4-hydroperoxy-2-methyl-1,3-dinitrooxybutan-2-ol	ISOP1N2OH3N4OOH	-
	3-hydroperoxy-2-methyl-3,4-dinitrooxybutan-1-ol	ISOP1N2N3OH4OOH	-
	3-hydroperoxy-2-methyl-1,4-dinitrooxybutan-2-ol	ISOP1OH2N3OOH4N	-
	4-hydroperoxy-3-methyl-1,3-dinitrooxybutan-2-ol	ISOP1N2OH3OOH4N	-
	1-hydroperoxy-2-methyl-3,4-dinitrooxybutan-2-ol	ISOP1OOH2N3OH4N	-
	2-hydroperoxy-3-methyl-3,4-dinitrooxybutan-1-ol	ISOP1OOH2OH3N4N	-
	2-hydroperoxy-2-methyl-3,4-dinitrooxybutan-1-ol	ISOP1N2N3OOH4OH	-
	3-methyl-3,4-dinitrooxybut-1-enal	ISOP1OH2OOH3N4N	-
	2-methyl-3,4-dinitrooxybut-1-enal	ISOP1N2N344CO	-
	1,3-dihydroperoxy-2-methyl-4-nitrooxybutan-2-ol	ISOP121CO3N4N	-
	3,4-dihydroperoxy-3-methyl-1-nitrooxybutan-2-ol	ISOP1OOH2OH3OOH4N	-
	2,3-dihydroperoxy-2-methyl-4-nitrooxybutan-1-ol	ISOP1OOH2OOH3OH4N	-
		ISOP1OH2OOH3OOH4N	-

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<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	1,3-dihydroperoxy-3-methyl-4-nitrooxybutan-2-ol	ISOPIN20OH3OH4OOH	-
	3,4-dihydroperoxy-2-methyl-1-nitrooxybutan-2-ol	ISOPIN20H3OOH4OOH	-
	2,3-dihydroperoxy-3-methyl-4-nitrooxybutan-1-ol	ISOPIN20OH3OOH4OH	-
	2-hydroperoxy-3-hydroxy-2-methyl-4-nitrooxybutanal	ISOP1CO2OOH3OH4N	INAHPCHO
	2-hydroperoxy-3-hydroxy-3-methyl-4-nitrooxybutanal	ISOP1N2OH3OOH4CO	-
	3-hydroperoxy-4-hydroxy-3-methyl-1-nitrooxybutan-2-one	ISOP1OH2OOH3CO4N	-
	3-hydroperoxy-1-hydroxy-3-methyl-4-nitrooxybutan-2-one	ISOPIN20OH3CO4OH	-
	3-methyl-4-nitrooxybut-1-enoic acid	ISOPIN4CO4OH	NC4CO2H
	2-methyl-4-nitrooxybut-1-enoic acid	ISOP1CO1OH4N	-
	3-methyl-4-nitrooxybut-1-enoic peracid	ISOPIN4CO4OOH	-
	2-methyl-4-nitrooxybut-1-enoic peracid	ISOP1CO1OOH4N	-
	3-hydroperoxy-3-methyl-4-nitrooxybut-1-enal	ISOPIN20OH344CO	-
	3-hydroperoxy-2-methyl-4-nitrooxybut-1-enal	ISOP121CO3OOH4N	-
	3-hydroxy-2-methyl-2,4-dinitrooxybutanal	ISOP1CO2N3OH4N	INANCHO
	3-hydroxy-3-methyl-2,4-dinitrooxybutanal	ISOPIN2OH3N4CO	INCNCHO
	4-hydroxy-3-methyl-1,3-dinitrooxybutan-2-one	ISOP1OH2N3CO4N	INANCO
	1-hydroxy-3-methyl-3,4-dinitrooxybutan-2-one	ISOPIN2N3CO4OH	INANCO
	peroxyacyl nitrate from (4,1)-ICN	ISOPIN4PAN	-
	peroxyacyl nitrate from (1,4)-ICN	ISOPIPAN4N	-
	ROOR from ISOPIN200 + ISOPIN400	ISOPIN200ISOPIN4	-
	ROOR from ISOPIN400 + ISOPIN400	ISOPIN400ISOPIN4	-
	ROOR from ISOP3004N + ISOPIN400	ISOP3004NISOPIN4	-
	ROOR from ISOPI004N + ISOPIN400	ISOPI004NISOPIN4	-
	ROOR from ISOPIN200 + ISOPIN200	ISOPIN200ISOPIN2	-
	ROOR from ISOP3004N + ISOPIN200	ISOP3004NISOPIN2	-
	ROOR from ISOPI004N + ISOPIN200	ISOPI004NISOPIN2	-
	peroxy radical from ISOPIN40 isomerization	<i>ISOPIN25_3004OH</i>	-
	alkoxy radical from ISOPIN25_3004OH	<i>ISOPIN25_304OH</i>	-
	3-hydroperoxy-4-hydroxy-2-nitrooxymethylbut-1-ene	ISOPIN25_30OH4OH	-
	3,4-dihydroxy-2-nitrooxymethylbut-1-ene	ISOPIN25_3OH4OH	-
	1-hydroxy-3-nitrooxymethylbut-3-en-2-one	ISOPIN25_3CO4OH	-
	4-hydroxy-3-nitrooxy-2-nitrooxymethylbut-1-ene	ISOPIN25_3N4OH	-
	ROOR from ISOPIN25_3004OH + ISOPIN400	ISOPIN25_3004OHISOPIN4	-

continued on next page

<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	ROOR from ISOPIN25_3OO4OH + ISOPIN2OO	ISOPIN25_3OO4OHISOPIN2	-
		MPAN	
	Methacryloyl peroxy nitrate	MPAN	MPAN
	energetically hot alkyl radical of MPAN	MPAN1OHx	-
	stabilized alkyl radical of MPAN	MPAN1OH	-
	peroxy radical from MPAN1OH	MPAN1OH2OO	-
	alkoxy radical from MPAN1OH2OO	MPAN1OH2O	-
	MPAN hydroperoxy nitrate	MPAN1OH2OOH	-
	Energetically hot HMML	HMMLx	-
	Hydroxymethyl methyl- α -lactone	HMML	HMML
	2-oxopropanoyl peroxy nitrate	CH3COCOON	CH3COPAN
		OZONE CHEMISTRY	
	C1 Stabilized Criegee	ciCH2OO	CH2OOE
	C4 Stabilized Criegee, structure MACR	ciMACROO	MACROOA
	C4 Stabilized Criegee, structure MVK	ciMVKOO	MVKOOA
	Hydroxymethyl hydroperoxide	HMHP	-
	Hydroperoxy methyl formate	HPMF	CHOOCH2OOH
	Formic anhydride	FAH	CHOOCHO
	Water dimer	H2Od	-
		METHACROLEIN DERIVATIVES	
	Methacrolein	MACR	MACR
	peroxy radical from MACR + OH (major)	MACR2OO3OH	MACRO2
	peroxy radical from MACR + OH (minor)	MACR2OH3OO	MACROHO2
	peroxy radical from MACR + OH (abstraction)	MACR1OO	MACO3
	2-hydroperoxy-3-hydroxy-2-methylpropanal	MACR2OOH3OH	MACROOH
	3-hydroperoxy-2-hydroxy-2-methylpropanal	MACR2OH3OOH	MACROHOOH
	Methacrylic acid	MACR1OH	MACO2H
	Methacrylic peracid	MACR1OOH	MACO3H
	2-nitrooxymethylacrolein	MACR3N	-
	peroxy radical from C4NVP2	MACR2OO3N	-
	2,3-dinitrooxy-2-methylpropanal	MACR2N3N	-
	3-hydroxy-2-methyl-2-nitrooxypropanal	MACR2N3OH	MACRNO3
	<i>continued on next page</i>		

<i>continued from previous page</i>	common / IUPAC name	our name	MCM name
	2-hydroxy-2-methyl-3-nitrooxypropanal	MACR2OH3N	MACRNB
	2-hydroperoxy-2-methyl-3-nitrooxypropanal	MACR2OOH3N	-
	2,3-dihydroperoxy-2-methylpropanal	MACR2OOH3OH	DHPMPAL
	2,3-dihydroxy-2-methylpropanal	MACR2OH3OH	MACROH
	2-hydroxy-2-methylpropane-1,3-dial	MACR2OH3CO	C3MDIALOH
	1-Hydroperoxy-2-methyl-2-propen-1-ol	MACR3OH3OOH	-
	2-hydroperoxy-2-methylpropane-1,3-dial	MACR2OOH3CO	C3MDIALOOH
	3-hydroxy-2-methylprop-2-enal	MACRENOL	HMAC
	2-methylpropene-1,3-dial	MACR3CO	-
	MVK DERIVATIVES		
	Methyl vinyl ketone	MVK	MVK
	peroxy radical from MVK + OH (major)	<i>MVK3OO4OH</i>	HMVKBO2
	peroxy radical from MVK + OH (minor)	<i>MVK3OH4OO</i>	HMVKAO2
	3,4-dihydroperoxybutan-2-one	MVK3OOH4OOH	DHPMEK
	3-hydroperoxy-4-hydroxybutan-2-one	MVK3OOH4OH	HMVKBOOH
	4-hydroperoxy-3-hydroxybutan-2-one	MVK3OH4OOH	HMVKAOOH
	2-Hydroperoxy-3-buten-2-ol	MVK3OH3OOH	-
	3-hydroxy-4-nitrooxybutan-2-one	MVK3OH4N	HMVKANO3
	4-hydroxy-3-nitrooxybutan-2-one	MVK3N4OH	MVKNO3
	3-hydroperoxy-4-nitrooxybutan-2-one	MVK3OOH4N	-
	3,4-dihydroxybutan-2-one	MVK3OH4OH	HO12CO3C4
	1-hydroxybutane-2,3-dione	MVK3CO4OH	BIACETOH
	1-nitrooxybutane-2,3-dione	MVK3CO4N	CO2C4NO3
	peroxy radical from C4NVPI	<i>MVK3OO4N</i>	-
	3,4-dinitrooxybutan-2-one	MVK3N4N	-
	2-hydroxy-3-oxobutanal	MVK3OH4CO	CO2H3CHO
	2-hydroperoxy-3-oxobutanal	MVK3OOH4CO	C4CO2OOH
	4-hydroxybut-3-en-2-one	MVKENOL	HVMK
	peroxy radical from MVKENOL + OH	<i>MVK3OO4OH4OH</i>	-
	3-oxobut-1-enal	MVK4CO	-
	peroxy radical from MVK4CO	<i>MVK3OO4CO4OH</i>	-
	SMALL PRODUCTS		

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common / IUPAC name	our name	MCM name
Formaldehyde	HCHO	HCHO
Glycolaldehyde	GLYC	HOCH2CHO
Methylglyoxal	MGLY	MGLYOX
Peroxyacetyl radical (PA)	CH3CO3	CH3CO3
Hydroxyperacetyl radical	HPA	HOCH2CO3
Nitrooxyperacetyl radical	NPA	NO3CH2CO3
Hydroxyacetone	HAC	ACETOL
Glyoxal	GLYX	GLYOX
Hydroperoxyacetone	HPAC	HYPERACET
Hydroperoxyethanal	HPETHNL	HCOCH2OOH
Methyl peroxy radical	CH3O	CH3O2
Methoxy radical	CH3OH	CH3O
Methanol	HCOOH	CH3OH
Formic acid	ETHLN	HCOOH
Ethanal nitrate	PROPNN	NO3CH2CHO
Propanone nitrate	CH3COOCH2	NOA
2-peroxypropene radical	PYRAC	CH3C2H2O2
Pyruvic acid	DHA	CH3COCO2H
1,1-dihydroxyacetone		-

Table I.3: Reactions included in the explicit isoprene mechanism, written in a syntax readable by the Kinetic PreProcessor (KPP). Each line is written "REACTANT + REACTANT = PRODUCTS : RATE COEFFICIENT ;\". Product and reactant names are given in Table I.2; rates coefficients are written in standard Arrhenius form unless they fall into one of the four alternative rate categories detailed in Chapter 4. Lines in bold denote section headings, while lines in italics denote epoxide formation reactions, for which alternate formulations can be found in Table I.4.

//OH Oxidation of Isoprene

ISOP + OH = ISOP1OHc : 2.7e-11*exp(390/T)*0.64*0.5;\

ISOP + OH = ISOP1OHt : 2.7e-11*exp(390/T)*0.64*0.5;\

ISOP + OH = ISOP4OHc : 2.7e-11*exp(390/T)*0.36*0.7;\

ISOP + OH = ISOP4OHt : 2.7e-11*exp(390/T)*0.36*0.3;\

//Reversible Addition of O2

ISOP4OHt + O2 = ISOP1OO4OHt : 5.3e-13;\

ISOP4OHt + O2 = ISOP3OO4OH : 7.1e-13;\

ISOP4OHc + O2 = ISOP1OO4OHc : 2.3e-13;\

ISOP4OHc + O2 = ISOP3OO4OH : 7.1e-13;\

ISOP1OHc + O2 = ISOP1OH4OOc : 1.4e-13;\

ISOP1OHc + O2 = ISOP1OH2OO : 7.8e-13;\

ISOP1OHt + O2 = ISOP1OH4OOt : 3.7e-13;\

ISOP1OHt + O2 = ISOP1OH2OO : 7.8e-13;\

ISOP1OO4OHt = ISOP4OHt : 2.08e14*exp(-9400/T);\

ISOP3OO4OH = ISOP4OHt : 2.49e15*exp(-10890/T);\

ISOP1OO4OHc = ISOP4OHc : 1.75e14*exp(-9054/T);\

ISOP3OO4OH = ISOP4OHc : 2.49e15*exp(-11112/T);\

ISOP1OH4OOc = ISOP1OHc : 1.79e14*exp(-8830/T);\

ISOP1OH2OO = ISOP1OHc : 2.22e15*exp(-10355/T);\

ISOP1OH4OOt = ISOP1OHt : 1.83e14*exp(-8930/T);\

ISOP1OH2OO = ISOP1OHt : 2.24e15*exp(-10865/T);\

// RO2 + NO

ISOP1OH2OO + NO = NO2 + MVK + HO2 + HCHO : k_alkoxy[2.7,350,1.190,6];\

ISOP1OH2OO + NO = ISOP1OH2N : k_nitrate[2.7,350,1.190,6];\

ISOP1OH4OOc + NO = NO2 + HO2 + ISOP1CO4OH : k_alkoxy[1.08,350,1.421,6];\

ISOP1OH4OOc + NO = NO2 + ISOP1CO2OO3OOH4OH : k_alkoxy[1.62,350,1.421,6];\

ISOP1OH4OOc + NO = ISOP1OH4Nc : k_nitrate[2.7,350,1.421,6];\

ISOP1OH4OOt + NO = NO2 + HO2 + ISOP1CO4OH : k_alkoxy[1.08,350,1.421,6];\

ISOP1OH4OOt + NO = NO2 + ISOP1CO2OO3OOH4OH : k_alkoxy[1.62,350,1.421,6];\

ISOP1OH4OOt + NO = ISOP1OH4Nt : k_nitrate[2.7,350,1.421,6];\

ISOP1CO2OO3OOH4OH = ISOP1CO2OOH3OO4OH : 3e6;\

ISOP1CO2OOH3OO4OH = ISOP1CO2OO3OOH4OH : 4e6;\

ISOP1CO2OO3OOH4OH + NO = NO2 + MGLY + GLYC + OH : k_alkoxy[2.7,350,22.270,9];\

ISOP1CO2OO3OOH4OH + NO = ISOP1CO2N3OOH4OH : k_nitrate[2.7,350,22.270,9];\

ISOP1CO2OO3OOH4OH = MVK3OOH4OH + CO + OH : 1e7*exp(-5000/T);\

ISOP1CO2OO3OOH4OH + HO2 = ISOP1CO2OOH3OOH4OH : 2.47e-13*exp(1300/T);\

ISOP1CO2OOH3OO4OH + NO = NO2 + MGLY + GLYC + OH : k_alkoxy[2.7,350,4.457,9];\

ISOP1CO2OOH3OO4OH + NO = ISOP1CO2OOH3N4OH : k_nitrate[2.7,350,4.457,9];\

ISOP1CO2OOH3OO4OH = MVK3OOH4OH + CO + OH : 4e8*exp(-5000/T);\

ISOP1CO2OOH3OO4OH + HO2 = ISOP1CO2OOH3OOH4OH : 2.47e-13*exp(1300/T);\

ISOP3OO4OH + NO = NO2 + MACR + HO2 + HCHO : k_alkoxy[2.7,350,1.297,6];\

ISOP3OO4OH + NO = ISOP3N4OH : k_nitrate[2.7,350,1.297,6];\

ISOP1OO4OHc + NO = NO2 + HO2 + ISOP1OH4CO : k_alkoxy[1.08,350,1.421,6];\

ISOP1OO4OHc + NO = NO2 + ISOP1OH2OOH3OO4CO : k_alkoxy[1.62,350,1.421,6];\

ISOP1OO4OHc + NO = ISOP1N4OHc : k_nitrate[2.7,350,1.421,6];\

ISOP1OO4OHt + NO = NO2 + HO2 + ISOP1OH4CO : k_alkoxy[1.08,350,1.421,6];\

ISOP1OO4OHt + NO = NO2 + ISOP1OH2OOH3OO4CO : k_alkoxy[1.62,350,1.421,6];\

ISOP1OO4OHt + NO = ISOP1N4OHt : k_nitrate[2.7,350,1.421,6];\

ISOP1OH2OOH3OO4CO = ISOP1OH2OO3OOH4CO : 4e6;\

ISOP1OH2OO3OOH4CO = ISOP1OH2OOH3OO4CO : 3e6;\

ISOP1OH2OOH3OO4CO + NO = NO2 + GLYX + HAC + OH : k_alkoxy[2.7,350,33.606,9];\

ISOP1OH2OOH3OO4CO + NO = ISOP1OH2OOH3N4CO : k_nitrate[2.7,350,33.606,9];\

ISOP1OH2OOH3OO4CO = MACR2OOH3OH + CO + OH : 1e7*exp(-5000/T);\

ISOP1OH2OOH3OO4CO + HO2 = ISOP1OH2OOH3OOH4CO : 2.47e-13*exp(1300/T);\

ISOP1OH2OO3OOH4CO + NO = NO2 + GLYX + HAC + OH : k_alkoxy[2.7,350,2.838,9];\

ISOP1OH2OO3OOH4CO + NO = ISOP1OH2N3OOH4CO : k_nitrate[2.7,350,2.838,9];\
 ISOP1OH2OO3OOH4CO = MACR2OOH3OH + CO + OH : 4e8*exp(-5000/T);\
 ISOP1OH2OO3OOH4CO + HO2 = ISOP1OH2OOH3OOH4CO : 2.47e-13*exp(1300/T);\
 ISOP1CO4OH + OH = MVK3OH4OH + CO + OH : 2.7e-11*exp(390/T);\
 ISOP1OH4CO + OH = MACR2OOH3OH + HO2 + CO : 2.7e-11*exp(390/T);\
 ISOP3CO4OH + OH = ISOP1OH2OO3CO4OH : 2.7e-11*exp(390/T);\
 ISOP1OH2OO3CO4OH + HO2 = ISOP1OH2OOH3CO4OH : 2.38e-13*exp(1300/T);\
 ISOP1OH2OO3CO4OH + NO = ISOP1OH2N3CO4OH : k_nitrate[2.7,350,13.338,8];\
 ISOP1OH2OO3CO4OH + NO = NO2 + HAC + HPA : k_alkoxy[2.7,350,13.338,8];\
//RO2 + Peroxy Radical
 ISOP1OH2OO + ISOP1OH2OO = MVK + MVK + HO2 + HO2 + HCHO + HCHO : 6.92e-14;\
 ISOP3OO4OH + ISOP3OO4OH = MACR + MACR + HO2 + HO2 + HCHO + HCHO : 5.74e-12*0.8;\
 ISOP3OO4OH + ISOP3OO4OH = ISOP3CO4OH + ISOP3OH4OH : 5.74e-12*0.2;\
 ISOP1OH2OO + ISOP3OO4OH = MVK + MACR + HO2 + HO2 + HCHO + HCHO : 3.08e-12*0.9;\
 ISOP1OH2OO + ISOP3OO4OH = ISOP1OH2OH + ISOP3CO4OH : 3.08e-12*0.1;\
 ISOP1OH2OO + ISOP1OO4OHc = MVK + HO2 + HCHO + HO2 + ISOP1OH4CO : 2.49e-12*0.805*0.4;\
 ISOP1OH2OO + ISOP1OO4OHc = MVK + HO2 + HCHO + ISOP1OH2OOH3OO4CO : 2.49e-12*0.805*0.6;\
 ISOP1OH2OO + ISOP1OO4OHc = ISOP1OH2OH + ISOP1CO4OH : 2.49e-12*(1-0.805);\
 ISOP1OH2OO + ISOP1OO4OHt = MVK + HO2 + HCHO + HO2 + ISOP1OH4CO : 2.49e-12*0.805*0.4;\
 ISOP1OH2OO + ISOP1OO4OHt = MVK + HO2 + HCHO + ISOP1OH2OOH3OO4CO : 2.49e-12*0.805*0.6;\
 ISOP1OH2OO + ISOP1OO4OHt = ISOP1OH2OH + ISOP1CO4OH : 2.49e-12*(1-0.805);\
 ISOP1OH2OO + ISOP1OH4OOc = MVK + HO2 + HCHO + HO2 + ISOP1CO4OH : 2.49e-12*0.805*0.4;\
 ISOP1OH2OO + ISOP1OH4OOc = MVK + HO2 + HCHO + ISOP1CO2OO3OOH4OH : 2.49e-12*0.805*0.6;\
 ISOP1OH2OO + ISOP1OH4OOc = ISOP1OH2OH + ISOP1OH4CO : 2.49e-12*(1-0.805);\
 ISOP1OH2OO + ISOP1OH4OOt = MVK + HO2 + HCHO + HO2 + ISOP1CO4OH : 2.49e-12*0.805*0.4;\
 ISOP1OH2OO + ISOP1OH4OOt = MVK + HO2 + HCHO + ISOP1CO2OO3OOH4OH : 2.49e-12*0.805*0.6;\
 ISOP1OH2OO + ISOP1OH4OOt = ISOP1OH2OH + ISOP1OH4CO : 2.49e-12*(1-0.805);\
 ISOP3OO4OH + ISOP1OO4OHc = MACR + HO2 + HCHO + HO2 + ISOP1OH4CO : 3.94e-12*0.705*0.4;\
 ISOP3OO4OH + ISOP1OO4OHc = MACR + HO2 + HCHO + ISOP1OH2OOH3OO4CO : 3.94e-12*0.705*0.6;\
 ISOP3OO4OH + ISOP1OO4OHc = ISOP3OH4OH + ISOP1CO4OH : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OO4OHc = ISOP1OH4OH + ISOP3CO4OH : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OO4OHt = MACR + HO2 + HCHO + HO2 + ISOP1OH4CO : 3.94e-12*0.705*0.4;\
 ISOP3OO4OH + ISOP1OO4OHt = MACR + HO2 + HCHO + ISOP1OH2OOH3OO4CO : 3.94e-12*0.705*0.6;\
 ISOP3OO4OH + ISOP1OO4OHt = ISOP3OH4OH + ISOP1CO4OH : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OO4OHt = ISOP1OH4OH + ISOP3CO4OH : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OH4OOc = MACR + HO2 + HCHO + HO2 + ISOP1CO4OH : 3.94e-12*0.705*0.4;\
 ISOP3OO4OH + ISOP1OH4OOc = MACR + HO2 + HCHO + ISOP1CO2OO3OOH4OH : 3.94e-12*0.705*0.6;\
 ISOP3OO4OH + ISOP1OH4OOc = ISOP3OH4OH + ISOP1OH4CO : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OH4OOc = ISOP1OH4OH + ISOP3CO4OH : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OH4OOt = MACR + HO2 + HCHO + HO2 + ISOP1CO4OH : 3.94e-12*0.705*0.4;\
 ISOP3OO4OH + ISOP1OH4OOt = MACR + HO2 + HCHO + ISOP1CO2OO3OOH4OH : 3.94e-12*0.705*0.6;\
 ISOP3OO4OH + ISOP1OH4OOt = ISOP3OH4OH + ISOP1OH4CO : 3.94e-12*(1-0.705)*0.5;\
 ISOP3OO4OH + ISOP1OH4OOt = ISOP1OH4OH + ISOP3CO4OH : 3.94e-12*(1-0.705)*0.5;\
 ISOP1OH2OO + CH3OO = MVK + CH3O + HO2 + HCHO : 2.00e-12*0.5;\
 ISOP1OH2OO + CH3OO = ISOP1OH2OH + HCHO : 2.00e-12*0.5;\
 ISOP3OO4OH + CH3OO = MACR + CH3O + HO2 + HCHO : 2.00e-12*0.5;\
 ISOP3OO4OH + CH3OO = ISOP3OH4OH + HCHO : 2.00e-12*0.25;\
 ISOP3OO4OH + CH3OO = ISOP3CO4OH + CH3OH : 2.00e-12*0.25;\
//RO2 + HO2 Radical
 HO2 + ISOP1OH2OO = ISOP1OH2OOH + O2 : 2.12e-13*exp(1300/T)*0.937;\
 HO2 + ISOP1OH2OO = MVK + OH + HO2 + HCHO : 2.12e-13*exp(1300/T)*0.063;\
 HO2 + ISOP3OO4OH = ISOP3OOH4OH + O2 : 2.12e-13*exp(1300/T)*0.937;\
 HO2 + ISOP3OO4OH = MACR + OH + HO2 + HCHO : 2.12e-13*exp(1300/T)*0.063;\
 HO2 + ISOP1OO4OHc = ISOP1OOH4OH + O2 : 2.12e-13*exp(1300/T);\
 HO2 + ISOP1OO4OHt = ISOP1OOH4OH + O2 : 2.12e-13*exp(1300/T);\
 HO2 + ISOP1OH4OOc = ISOP1OH4OOH + O2 : 2.12e-13*exp(1300/T);\
 HO2 + ISOP1OH4OOt = ISOP1OH4OOH + O2 : 2.12e-13*exp(1300/T);\
//Peroxy Isomerization
 ISOP1OH4OOc = ISOP1CO4OOHc + HO2 : 0.34*k_tunneling[5.47e15,-12200,1e8];\
 ISOP1OH4OOc = ISOP1CO2OO3OOH4OOH : 0.66*k_tunneling[5.47e15,-12200,1e8];\
 ISOP1CO2OO3OOH4OOH = ISOP1CO2OOH3OO4OOH : 3e6;\
 ISOP1CO2OO3OOH4OOH = ISOP1CO2OOH3OOH4OO : 2e6;\
 ISOP1CO2OOH3OO4OOH = ISOP1CO2OO3OOH4OOH : 4e6;\
 ISOP1CO2OOH3OO4OOH = ISOP1CO2OOH3OOH4OO : 2e6;\
 ISOP1CO2OOH3OOH4OO = ISOP1CO2OO3OOH4OOH : 4e6;\
 ISOP1CO2OOH3OOH4OO = ISOP1CO2OOH3OO4OOH : 3e6;\
 ISOP1CO2OO3OOH4OOH = MVK3OOH4OOH + OH + CO : 1e7*exp(-5000/T);\
 ISOP1CO2OOH3OO4OOH = MVK3OOH4OOH + OH + CO : 4e8*exp(-5000/T);\
 ISOP1CO2OO3OOH4OOH = MVK3OOH4OOH + OH + CO : 1e8*exp(-5000/T);\
 ISOP1CO2OO3OOH4OOH + NO = ISOP1CO2N3OOH4OOH : k_nitrate[2.7,350,20.511,10];\
 ISOP1CO2OO3OOH4OOH + NO = NO2 + CO + HO2 + MVK3OOH4OOH : k_alkoxy[0.54,350,20.511,10];\
 ISOP1CO2OO3OOH4OOH + NO = NO2 + OH + MGLY + HPETHNL : k_alkoxy[2.16,350,20.511,10];\
 ISOP1CO2OO3OOH4OOH + HO2 = OH + OH + MGLY + HPETHNL : 0.58*2.54e-13*exp(1300/T);

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ISOP1CO2OO3OOH4OOH + HO2 = OH + CO + HO2 + MVK3OOH4OOH : 0.15*2.54e-13*exp(1300/T);\
ISOP1CO2OO3OOH4OOH + HO2 = ISOP1CO2OOH3OOH4OOH : 0.27*2.54e-13*exp(1300/T);\
ISOP1CO2OOH3OO4OOH + NO = ISOP1CO2OOH3N4OOH : k_nitrate[2.7,350,7.425,10];\
ISOP1CO2OOH3OO4OOH + NO = NO2 + CO + HO2 + MVK3OOH4OOH : k_alkoxy[0.54,350,7.425,10];\
ISOP1CO2OOH3OO4OOH + NO = NO2 + OH + MGLY + HPETHNL : k_alkoxy[2.16,350,7.425,10];\
ISOP1CO2OOH3OO4OOH + HO2 = OH + OH + MGLY + HPETHNL : 0.58*2.54e-13*exp(1300/T);\
ISOP1CO2OOH3OO4OOH + HO2 = OH + CO + HO2 + MVK3OOH4OOH : 0.15*2.54e-13*exp(1300/T);\
ISOP1CO2OOH3OO4OOH + HO2 = ISOP1CO2OOH3OOH4OOH : 0.27*2.54e-13*exp(1300/T);\
ISOP1CO2OOH3OOH4OO + NO = ISOP1CO2OOH3OOH4N : k_nitrate[2.7,350,5.854,10];\
ISOP1CO2OOH3OOH4OO + NO = OH + NO2 + CH2O + MACR2OOH3CO : k_alkoxy[2.7,350,5.854,10];\
ISOP1CO2OOH3OOH4OO + HO2 = ISOP1CO2OOH3OOH4OOH : 2.54e-13*exp(1300/T);\
ISOP1OO4OHc = ISOP1OOH4COc + HO2 : 0.34*k_tunneling[2.40e9,-7160,1e8];\
ISOP1OO4OHc = ISOP1OOH2OOH3OO4CO : 0.66*k_tunneling[2.40e9,-7160,1e8];\
ISOP1OOH2OOH3OO4CO = ISOP1OOH2OO3OOH4CO : 4e6;\
ISOP1OOH2OOH3OO4CO = ISOP1OO2OOH3OOH4CO : 2e6;\
ISOP1OOH2OO3OOH4CO = ISOP1OOH2OOH3OO4CO : 3e6;\
ISOP1OOH2OO3OOH4CO = ISOP1OO2OOH3OOH4CO : 2e6;\
ISOP1OO2OOH3OOH4CO = ISOP1OOH2OOH3OO4CO : 3e6;\
ISOP1OO2OOH3OOH4CO = ISOP1OOH2OO3OOH4CO : 4e6;\
ISOP1OOH2OOH3OO4CO = MACR2OOH3OOH + OH + CO : 1e7*exp(-5000/T);\
ISOP1OOH2OO3OOH4CO = MACR2OOH3OOH + OH + CO : 4e8*exp(-5000/T);\
ISOP1OO2OOH3OOH4CO = MACR2OOH3OOH + OH + CO : 1e8*exp(-5000/T);\
ISOP1OOH2OOH3OO4CO + NO = ISOP1OOH2OOH3N4CO : k_nitrate[2.7,350,30.981,10];\
ISOP1OOH2OOH3OO4CO + NO = NO2 + CO + HO2 + MACR2OOH3OOH : k_alkoxy[0.54,350,30.981,10];\
ISOP1OOH2OOH3OO4CO + NO = NO2 + OH + GLYX + HPAC : k_alkoxy[2.16,350,30.981,10];\
ISOP1OOH2OOH3OO4CO + HO2 = HO2 + OH + GLYX + HPAC : 0.58*2.54e-13*exp(1300/T);\
ISOP1OOH2OOH3OO4CO + HO2 = HO2 + CO + HO2 + MACR2OOH3OOH : 0.15*2.54e-13*exp(1300/T);\
ISOP1OOH2OOH3OO4CO + HO2 = ISOP1OOH2OOH3OOH4CO : 0.27*2.54e-13*exp(1300/T);\
ISOP1OOH2OO3OOH4CO + NO = ISOP1OOH2N3OOH4CO : k_nitrate[2.7,350,4.808,10];\
ISOP1OOH2OO3OOH4CO + NO = NO2 + CO + HO2 + MACR2OOH3OOH : k_alkoxy[0.54,350,4.808,10];\
ISOP1OOH2OO3OOH4CO + NO = NO2 + OH + GLYX + HPAC : k_alkoxy[2.16,350,4.808,10];\
ISOP1OOH2OO3OOH4CO + HO2 = HO2 + OH + GLYX + HPAC : 0.58*2.54e-13*exp(1300/T);\
ISOP1OOH2OO3OOH4CO + HO2 = HO2 + CO + HO2 + MACR2OOH3OOH : 0.15*2.54e-13*exp(1300/T);\
ISOP1OOH2OO3OOH4CO + NO = ISOP1N2OOH3OOH4CO : k_nitrate[2.7,350,5.854,10];\
ISOP1OO2OOH3OOH4CO + NO = NO2 + OH + CH2O + MVK3OOH4CO : k_alkoxy[2.7,350,5.854,10];\
ISOP1OO2OOH3OOH4CO + HO2 = ISOP1OOH2OOH3OOH4CO : 2.54e-13*exp(1300/T);\
ISOP1OH2OO = HCHO + OH + MVK : 1.04e11*exp(-9746/T);\
ISOP3OO4OH = MACR + OH + HCHO : 1.88e11*exp(-9752/T);\
//MVK\
MVK + OH = MVK3OO4OH : 2.6e-12*exp(610/T)*0.76;\
MVK + OH = MVK3OH4OO : 2.6e-12*exp(610/T)*0.24;\
MVK3OO4OH + HO2 = CH3CO3 + GLYC + OH : 2.12e-13*exp(1300/T)*0.48;\
MVK3OO4OH + HO2 = MVK3CO4OH + OH + HO2 : 2.12e-13*exp(1300/T)*0.34;\
MVK3OO4OH + HO2 = MVK3OOH4OH : 2.12e-13*exp(1300/T)*0.18;\
MVK3OH4OO + HO2 = MVK3OH4OOH : 2.12e-13*exp(1300/T)*0.83;\
MVK3OH4OO + HO2 = MGLY + HCHO + OH + HO2 : 2.12e-13*exp(1300/T)*0.17;\
MVK3OOH4OH = CH3CO3 + GLYC + OH : SUN*3e-5;\
MVK3OO4OH + NO = CH3CO3 + GLYC + NO2 : k_alkoxy[2.7,350,6.161,6];\
MVK3OO4OH + NO = MVK3N4OH : k_nitrate[2.7,350,6.161,6];\
MVK3OH4OO + NO = MGLY + HCHO + HO2 + NO2 : k_alkoxy[2.7,350,2.531,6];\
MVK3OH4OO + NO = MVK3OH4N : k_nitrate[2.7,350,2.531,6];\
MVK3N4OH = CH3CO3 + GLYC + NO2 : SUN*6.46e-5;\
MVK3OH4N = CH3CO3 + ETHLN + HO2 : SUN*4.21e-5;\
//MACR\
MACR + OH = MACR2OO3OH : 8.0e-12*exp(380/T)*0.53;\
MACR + OH = MACR2OH3OO : 8.0e-12*exp(380/T)*0.02;\
MACR + OH = MACR1OO : 2.7e-12*exp(470/T);\
MACR2OO3OH + HO2 = MACR2OOH3OH : 2.12e-13*exp(1300/T)*0.41;\
MACR2OO3OH + HO2 = HAC + CO + HO2 + OH + O2 : 2.12e-13*exp(1300/T)*0.59*0.86;\
MACR2OO3OH + HO2 = MGLY + HCHO + OH + O2 : 2.12e-13*exp(1300/T)*0.59*0.14;\
MACR2OH3OO + HO2 = MACR2OH3OOH : 2.12e-13*exp(1300/T)*0.83;\
MACR2OH3OO + HO2 = MGLY + HCHO + HO2 + OH + O2 : 2.12e-13*exp(1300/T)*0.17;\
MACR1OO + HO2 = MACR1OOH : 1.93e-13*exp(1300/T)*0.40;\
MACR1OO + HO2 = CH3COOCH2 + O2 + CO2 + OH : 1.93e-13*exp(1300/T)*0.40;\
MACR1OO + HO2 = MACR1OH + O3 : 1.93e-13*exp(1300/T)*0.20;\
MACR2OO3OH + NO = HAC + CO + HO2 + NO2 : k_alkoxy[2.322,350,2.985,6];\
MACR2OO3OH + NO = MGLY + HCHO + NO2 : k_alkoxy[0.378,350,2.985,6];\
MACR2OO3OH + NO = MACR2N3OH : k_nitrate[2.7,350,2.985,6];\
MACR2OH3OO + NO = MGLY + HCHO + HO2 + NO2 : k_alkoxy[2.7,350,2.985,6];\
MACR2OH3OO + NO = MACR2OH3N : k_nitrate[2.7,350,2.985,6];\
MACR1OO + NO = CH3COOCH2 + CO2 + NO2 : 8.7e-12*exp(290/T);\
MACR1OO + NO2 + M = MPAN + M : k_troe[k_0 = 2.133e-28*(T/300)^(-7.1), k_inf = 1.2e-11*(T/300)^(-0.9), Fc = 0.3];\

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MPAN + M = MACR1OO + NO2 + M : $k_{\text{troe}}[k_0 = 3.871e-3 * \exp(-12100/T), k_{\text{inf}} = 5.4e16 * \exp(-13830/T), Fc = 0.3]; \backslash$
 MACR2OO3OH = HAC + CO + OH : $2.9e7 * \exp(-5297/T); \backslash$
 MACR2OH3OO = HPAC + CO + HO2 : $4e8 * \exp(-5000/T); \backslash$
//MPAN
 MPAN + OH = MPAN1OHx : $2.9e-11; \backslash$
 MPAN1OHx = MPAN1OH2OO : $1e7; \backslash$
 MPAN1OHx = HMMLx : $4e9; \backslash$
 MPAN1OHx = MPAN1OH : $8.18e7; \backslash$
 MPAN1OH = HMMLx : $1e3; \backslash$
 MPAN1OH = MPAN1OH2OO : $1e7; \backslash$
 HMMLx = HMML + NO3 : $1E8 * 0.75; \backslash$
 HMMLx = HAC + CO + NO3 : $1E8 * 0.25; \backslash$
 MPAN1OH2OO + NO = MPAN1OH2O + NO2 : $2.7E-12 * \exp(350/T); \backslash$
 MPAN1OH2OO + HO2 = MPAN1OH2OOH : $2.6e-13 * \exp(1300/T) * 0.1; \backslash$
 MPAN1OH2OO + HO2 = MPAN1OH2O + OH : $2.6e-13 * \exp(1300/T) * 0.9; \backslash$
 MPAN1OH2O = HAC + CO2 + NO3 : $1E8 * 0.4; \backslash$
 MPAN1OH2O = HO2 + HCHO + CH3COCOON : $1E8 * 0.6; \backslash$
//ISOPOOH
 ISOP1OH2OOH + OH = ISOP1OH2OOH3R4OH : $1.7e-11 * \exp(390/T) * 0.95; \backslash$
 ISOP1OH2OOH3R4OH + O2 = ISOP1OH2OOH3OO4OH : $1e-14; \backslash$
 ISOP1OH2OOH3R4OH = ISOP1OH23O4OH : $4.4e5 * 0.67; \backslash$
 ISOP1OH2OOH3R4OH = ISOP1OH23O4OHc : $4.4e5 * 0.33; \backslash$
 ISOP3OOH4OH + OH = ISOP1OH2R3OOH4OH : $3.0e-11 * \exp(390/T) * 0.95; \backslash$
 ISOP1OH2R3OOH4OH + O2 = ISOP1OH2OO3OOH4OH : $1e-14; \backslash$
 ISOP1OH2R3OOH4OH = ISOP1OH23O4OH : $4.4e5 * 0.68; \backslash$
 ISOP1OH2R3OOH4OH = ISOP1OH23O4OHc : $4.4e5 * 0.32; \backslash$
 ISOP1OOH4OH + OH = ISOP12O3OH4OH + OH : $2.9e-11 * \exp(390/T); \backslash$
 ISOP1OH4OOH + OH = ISOP1OH2OOH3OH4CO + OH : $2.9e-11 * \exp(390/T); \backslash$
 ISOP1OH2OOH + OH = ISOP1OH2OOH3OH4OO : $1.7e-11 * \exp(390/T) * 0.05; \backslash$
 ISOP1OH2OOH3OH4OO = ISOP1OH2OO3OH4OOH : $3e6; \backslash$
 ISOP1OH2OO3OH4OOH = ISOP1OH2OOH3OH4OO : $7e6; \backslash$
 ISOP1OH2OOH3OH4OO + NO = GLYC + HAC + NO2 + OH : $k_{\text{alkoxy}}[2.7,350,3.485,9]; \backslash$
 ISOP1OH2OOH3OH4OO + NO = ISOP1OH2OOH3OH4N : $k_{\text{nitrate}}[2.7,350,3.485,9]; \backslash$
 ISOP1OH2OO3OH4OOH + NO = HPETHNL + HAC + NO2 + HO2 : $k_{\text{alkoxy}}[2.7,350,1.450,9]; \backslash$
 ISOP1OH2OO3OH4OOH + NO = ISOP1OH2N3OH4OOH : $k_{\text{nitrate}}[2.7,350,1.450,9]; \backslash$
 ISOP1OH2OOH3OH4OO + HO2 = ISOP1OH2OOH3OH4OOH : $2.47e-13 * \exp(1300/T); \backslash$
 ISOP1OH2OO3OH4OOH + HO2 = ISOP1OH2OOH3OH4OOH : $2.47e-13 * \exp(1300/T); \backslash$
 ISOP1OH2OO3OH4OOH = ISOP1OH2OOH3OH4CO : $3.75e13 * \exp(-10000/T); \backslash$
 ISOP3OOH4OH + OH = ISOP1OO2OH3OOH4OH : $3.0e-11 * \exp(390/T) * 0.05; \backslash$
 ISOP1OO2OH3OOH4OH = ISOP1OOH2OH3OO4OH : $3e6; \backslash$
 ISOP1OOH2OH3OO4OH = ISOP1OO2OH3OOH4OH : $7e6; \backslash$
 ISOP1OO2OH3OOH4OH + NO = HAC + GLYC + NO2 + OH : $k_{\text{alkoxy}}[1.89,350,3.485,9]; \backslash$
 ISOP1OO2OH3OOH4OH + NO = ISOP1N2OH3OOH4OH : $k_{\text{nitrate}}[1.89,350,3.485,9]; \backslash$
 ISOP1OOH2OH3OO4OH + NO = HPAC + GLYC + NO2 + HO2 : $k_{\text{alkoxy}}[0.81,350,2.375,9]; \backslash$
 ISOP1OOH2OH3OO4OH + NO = ISOP1OOH2OH3N4OH : $k_{\text{nitrate}}[0.81,350,2.375,9]; \backslash$
 ISOP1OO2OH3OOH4OH + HO2 = ISOP1OOH2OH3OOH4OH : $2.47e-13 * \exp(1300/T); \backslash$
 ISOP1OOH2OH3OO4OH + HO2 = ISOP1OOH2OH3OOH4OH : $2.47e-13 * \exp(1300/T); \backslash$
 ISOP1OOH2OH3OO4OH = ISOP1CO2OH3OOH4OH : $3.75e13 * \exp(-10000/T); \backslash$
 ISOP1OH2OOH3OO4OH = ISOP1OH2OO3OOH4OH : $4e6; \backslash$
 ISOP1OH2OO3OOH4OH = ISOP1OH2OOH3OO4OH : $3e6; \backslash$
 ISOP1OH2OOH3OO4OH + NO = ISOP1OH2OOH3N4OH : $k_{\text{nitrate}}[2.7,350,4.457,9]; \backslash$
 ISOP1OH2OOH3OO4OH + NO = GLYC + HAC + NO2 + OH : $k_{\text{alkoxy}}[2.7,350,4.457,9]; \backslash$
 ISOP1OH2OOH3OO4OH + HO2 = ISOP1OH2OOH3OOH4OH : $2.47e-13 * \exp(1300/T); \backslash$
 ISOP1OH2OOH3OO4OH = ISOP1OH12O3OOH4OH : $1e14 * \exp(-10000/T); \backslash$
 ISOP1OH2OO3OOH4OH + NO = ISOP1OH2N3OOH4OH : $k_{\text{nitrate}}[2.7,350,2.838,9]; \backslash$
 ISOP1OH2OO3OOH4OH + NO = HAC + GLYC + NO2 + OH : $k_{\text{alkoxy}}[2.7,350,2.838,9]; \backslash$
 ISOP1OH2OO3OOH4OH + HO2 = ISOP1OH2OOH3OOH4OH : $2.47e-13 * \exp(1300/T); \backslash$
 ISOP1OH2OO3OOH4OH = ISOP1OH2OOH34O4OH : $1e14 * \exp(-10000/T); \backslash$
 ISOP1OH2OOH + OH = ISOP1OH2OO : $4.6e-12 * \exp(200/T); \backslash$
 ISOP1OH2OOH + OH = ISOP1CO2OOH + HO2 : $1.5e-12 * \exp(200/T) * 0.5; \backslash$
 ISOP1OH2OOH + OH = ISOP1OH12O + OH : $1.5e-12 * \exp(200/T) * 0.5; \backslash$
 ISOP3OOH4OH + OH = ISOP3OO4OH : $2.1e-12 * \exp(200/T); \backslash$
 ISOP3OOH4OH + OH = ISOP3CO4OH + OH : $2.0e-12 * \exp(200/T) * 0.32; \backslash$
 ISOP3OOH4OH + OH = ISOP3OOH4CO + HO2 : $2.0e-12 * \exp(200/T) * 0.68; \backslash$
 ISOP1OH2OOH = MVK + HCHO + HO2 + OH : $SUN * 6.5e-6; \backslash$
 ISOP3OOH4OH = MACR + HCHO + HO2 + OH : $SUN * 6.5e-6; \backslash$
//IEPOX
 ISOP1OH23O4OHc + OH = ISOP1OH23O4R4OHc : $0.168 * 5.82e-11 * \exp(-400/T); \backslash$
 ISOP1OH23O4R4OHc + O2 = ISOP1OH23O4CO + H2O + HO2 : $1e-14; \backslash$
 ISOP1OH23O4R4OHc = HAC + GLYX + OH : $0.63 * 0.168 * 1.752e5; \backslash$
 ISOP1OH23O4R4OHc = MACR2OH3OH + OH + CO : $0.37 * 0.168 * 1.752e5; \backslash$
 ISOP1OH23O4OHc + OH = ISOP1OH1R23O4OHc : $0.752 * 5.82e-11 * \exp(-400/T); \backslash$
 ISOP1OH1R23O4OHc + O2 = ISOP1CO23O4OH + H2O + HO2 : $1e-14; \backslash$

$ISOP1OH1R23O4OHc = GLYC + MGLY + OH : 0.287*0.752*1.752e5;$
 $ISOP1OH1R23O4OHc = MVK3OH4OH + OH + CO : 0.713*0.752*1.752e5;$
 $ISOP1OH23O4OHc + OH = MVK3CO4OH + OH + HCHO : 0.08*5.82e-11*exp(-400/T);$
 $ISOP1OH23O4OHt + OH = ISOP1OH23O4R4OHt : 0.31*3.75e-11*exp(-400/T);$
 $ISOP1OH23O4R4OHt + O2 = ISOP1OH23O4CO + H2O + HO2 : 1e-14;$
 $ISOP1OH23O4R4OHt = HAC + GLYX + OH : 0.63*0.31*2.15e5;$
 $ISOP1OH23O4R4OHt = MACR2OH3OH + OH + CO : 0.37*0.31*2.15e5;$
 $ISOP1OH23O4OHt + OH = ISOP1OH1R23O4OHt : 0.62*3.75e-11*exp(-400/T);$
 $ISOP1OH1R23O4OHt + O2 = ISOP1CO23O4OH + H2O + HO2 : 1e-14;$
 $ISOP1OH1R23O4OHt = GLYC + MGLY + OH : 0.287*0.62*2.15e5;$
 $ISOP1OH1R23O4OHt = MVK3OH4OH + OH + CO : 0.713*0.62*2.15e5;$
 $ISOP1OH23O4OHt + OH = MVK3CO4OH + OH + HCHO : 0.07*3.75e-11*exp(-400/T);$
 $ISOP1OH2OH34O + OH = ISOP1CO2OH34O + HO2 : 3.22e-11*exp(-400/T);$
 $ISOP12O3OH4OH + OH = ISOP12O3OH4CO + HO2 : 0.2*3.22e-11*exp(-400/T);$
 $ISOP12O3OH4OH + OH = ISOP12O3OH3R4OH : 0.8*3.22e-11*exp(-400/T);$
 $ISOP12O3OH3R4OH + O2 = ISOP12O3CO4OH + HO2 : 0.33*1e-14;$
 $ISOP12O3OH3R4OH + O2 = ISOP1OH3OH4CO + HO2 : 0.67*1e-14;$
 $ISOP12O3OH3R4OH = ISOP1OH2OO3CO4OH : 3.45e4;$
//C4 dihydroxycarbonyls
 $MVK3OH4OH + OH = MVK3OH4CO + HO2 : 0.4*8.7e-12*exp(70/T);$
 $MVK3OH4OH + OH = MVK3CO4OH + HO2 : 0.6*8.7e-12*exp(70/T);$
 $MVK3OH4CO + OH = OH + MGLY + CO2 : 5e-12*exp(470/T);$
 $MVK3OH4CO = CO + HO2 + HO2 + MGLY : 0.5*2.5e-4*SUN;$
 $MVK3OH4CO = GLYX + HO2 + CH3CO3 : 0.5*2.5e-4*SUN;$
 $MVK3CO4OH + OH = CO + CO + HO2 + CH3CO3 : 2e-12*exp(70/T);$
 $MVK3CO4OH = CO + HO2 + CH2O + CH3CO3 : 2.5e-4*SUN;$
 $MACR2OH3OH + OH = MACR2OH3CO + HO2 : 0.16*2.4e-11*exp(70/T);$
 $MACR2OH3OH + OH = HAC + OH + CO2 : 0.84*2.4e-11*exp(70/T);$
 $MACR2OH3CO + OH = CO2 + OH + MGLY : 5e-12*exp(470/T);$
//HPALD
 $ISOP1CO4OOHc = MVKENOL + OH + OH + CO : 0.552*0.58*SUN*4e-4;$
 $ISOP1CO4OOHc = C4HVP1 + OH + CO : 0.224*0.58*SUN*4e-4;$
 $ISOP1CO4OOHc = ISOP1CO4CO + HO2 + OH : 0.112*0.58*SUN*4e-4;$
 $ISOP1CO4OOHc = MACR2OOH3CO + OH + OH + CO : 0.019*0.58*SUN*4e-4;$
 $ISOP1CO4OOHc = MVK3OOH4CO + OH + OH + CO : 0.093*0.58*SUN*4e-4;$
 $ISOP1OOH4COc = MACRENOL + OH + OH + CO : 0.455*0.55*SUN*4e-4;$
 $ISOP1OOH4COc = C4HVP2 + OH + CO : 0.182*0.55*SUN*4e-4;$
 $ISOP1OOH4COc = ISOP1CO4CO + HO2 + OH : 0.182*0.55*SUN*4e-4;$
 $ISOP1OOH4COc = MACR2OOH3CO + OH + OH + CO : 0.031*0.55*SUN*4e-4;$
 $ISOP1OOH4COc = MVK3OOH4CO + OH + OH + CO : 0.151*0.55*SUN*4e-4;$
 $MVKENOL + OH = HO2 + MVK3OH4CO : 0.3*3.35e-12*exp(983/T);$
 $MVKENOL + OH = MVK3OO4OH4OH : 0.7*3.35e-12*exp(983/T);$
 $MVKENOL = CH3CO3 + GLYX + OH : 0.5*2.5e-4*SUN;$
 $MVKENOL = MGLY + HO2 + CO + OH : 0.5*2.5e-4*SUN;$
 $MVK3OO4OH4OH + NO = NO2 + HO2 + HCOOH + MGLY : 2.7E-12*exp(350/T);$
 $MVK3OO4OH4OH + HO2 = OH + HO2 + HCOOH + MGLY : 2.26e-13*exp(1300/T);$
 $MACRENOL + OH = DHA + CO + OH : 3.35e-12*exp(983/T);$
 $DHA + OH = HO2 + PYRAC : 8e-12*exp(70/T);$
 $MACRENOL = MACR3CO + OH + OH : 2.5e-4*SUN;$
 $MACR3CO + OH = PYRAC + OH + CO : 2.7e-11*exp(390/T);$
 $C4HVP1 + NO = NO2 + MVK3OO4OH : 2.7E-12*exp(350/T);$
 $C4HVP1 + HO2 = OH + MVK3OO4OH : 1.93e-13*exp(1300/T);$
 $C4HVP1 + NO2 = MVK3N4OH : 9e-12;$
 $C4HVP2 + NO = NO2 + MACR2OO3OH : 2.7E-12*exp(350/T);$
 $C4HVP2 + HO2 = OH + MACR2OO3OH : 1.93e-13*exp(1300/T);$
 $C4HVP2 + NO2 = MACR2N3OH : 9e-12;$
 $MACR2OOH3CO = OH + MGLY + HO2 + CO : 2.5e-4*SUN;$
 $MVK3OOH4CO = OH + GLYX + CH3CO3 : 2.5e-4*SUN;$
 $ISOP1CO4OOHc + OH = ISOP1CO4CO + OH : 7.5e-12*exp(20/T);$
 $ISOP1CO4OOHc + OH = ISOP1CO4OOc : 2.0e-12*exp(200/T);$
 $ISOP1CO4OOHc + OH = ISOP1CO2OO3OH4OOH : 2.0e-12*exp(650/T);$
 $ISOP1CO4OOHc + OH = ISOP1CO2OH3R4OOH : 1.0e-12*exp(650/T);$
 $ISOP1CO2OH3R4OOH + O2 = ISOP1CO2OH3OO4OOH : 1e-14;$
 $ISOP1CO2OH3R4OOH = ISOP1CO2OH34O : 5.2e4;$
 $ISOP1CO4OOHc + OH = ISOP1CO3R4OOH : 3.8e-12*exp(400/T);$
 $ISOP1CO3R4OOH + O2 = ISOP1CO1OOH4CO : 1e-14*0.125;$
 $ISOP1CO3R4OOH + O2 = ISOP12ICO3OO4OOH : 1e-14*0.875;$
 $ISOP1CO3R4OOH = ISOP12ICO34O : 1.3e4;$
 $ISOP1CO2OH3OO4OOH = MVK3OOH4OOH + CO2 + HO2 : 4e8*exp(-5000/T);$
 $ISOP1CO2OH3OOH4OO = MVK3OOH4OOH + CO2 + HO2 : 1e8*exp(-5000/T);$
 $ISOP1CO2OH3OO4OOH = ISOP1CO2OH3OOH4OO : 2e6;$
 $ISOP1CO2OH3OOH4OO = ISOP1CO2OH3OO4OOH : 3e6;$
 $ISOP1CO2OO3OH4OOH = MVK3OH4OOH + CO + OH : 1e7*exp(-5000/T);$

ISOP1CO2OOH3OH4OO = MVK3OH4OOH + CO + OH : 1e8*exp(-5000/T);\
 ISOP1CO2OO3OH4OOH = ISOP1CO2OOH3OH4OO : 2e6;\
 ISOP1CO2OOH3OH4OO = ISOP1CO2OO3OH4OOH : 4e6;\
 ISOP1CO4OOc = ISOP1CO2OO : 10;\
 ISOP1CO2OO = MVK + OH + CO : 1e7*exp(-5000/T);\
 ISOP1CO4OOc = ISOP1CO3R4OOH : 10;\
 ISOP121CO3OO4OOH + NO = OH + CH2O + NO2 + MACR3CO : 2.7E-12*exp(350/T);\
 ISOP121CO3OO4OOH + HO2 = OH + OH + CH2O + MACR3CO : 2.38e-12*exp(1300/T);\
 ISOP1OOH4COc + OH = ISOP1CO4CO + OH : 7.5e-12*exp(20/T);\
 ISOP1OOH4COc + OH = ISOP1OO4COc : 2.0e-12*exp(200/T);\
 ISOP1OOH4COc + OH = ISOP1OOH2OH3OO4CO : 1.0e-12*exp(650/T);\
 ISOP1OOH4COc + OH = ISOP1OOH2R3OH4CO : 2.0e-12*exp(650/T);\
 ISOP1OOH2R3OH4CO + O2 = ISOP1OOH2OO3OH4CO : 1e-14;\
 ISOP1OOH2R3OH4CO = ISOP12O3OH4CO : 5.2e4;\
 ISOP1OOH4COc + OH = ISOP1OOH2R4CO : 3.8e-12*exp(400/T);\
 ISOP1OOH2R4CO + O2 = ISOP1OOH2OO344CO : 1e-14*0.875;\
 ISOP1OOH2R4CO + O2 = ISOP1CO4CO4OOH : 1e-14*0.125;\
 ISOP1OOH2R4CO = ISOP12O344CO : 1.3e4;\
 ISOP1OOH2OH3OO4CO = MACR2OH3OOH + OH + CO : 1e7*exp(-5000/T);\
 ISOP1OO2OH3OOH4CO = MACR2OH3OOH + OH + CO : 1e8*exp(-5000/T);\
 ISOP1OOH2OH3OO4CO = ISOP1OO2OH3OOH4CO : 2e6;\
 ISOP1OO2OH3OOH4CO = ISOP1OOH2OH3OO4CO : 3e6;\
 ISOP1OOH2OO3OH4CO = MACR2OOH3OOH + CO + HO2 : 4e8*exp(-5000/T);\
 ISOP1OO2OOH3OH4CO = MACR2OOH3OOH + CO + HO2 : 1e8*exp(-5000/T);\
 ISOP1OOH2OO3OH4CO = ISOP1OO2OOH3OH4CO : 2e6;\
 ISOP1OO2OOH3OH4CO = ISOP1OOH2OO3OH4CO : 4e6;\
 ISOP1OO4COc = ISOP3OO4CO : 10;\
 ISOP3OO4CO = MACR + CO + OH : 2.9e7*exp(-5297/T);\
 ISOP1OO4COc = ISOP1OOH2R4CO : 10;\
 ISOP1OOH2OO344CO + NO = OH + OH + CH2O + MVK4CO : 2.7E-12*exp(350/T);\
 ISOP1OOH2OO344CO + HO2 = OH + OH + CH2O + MVK4CO : 2.38e-12*exp(1300/T);\
 MVK4CO + OH = MVK3OO4CO4OH : 2.7e-11*exp(390/T);\
 MVK3OO4CO4OH + NO = NO2 + CO2 + HO2 + MGLY : 2.7E-12*exp(350/T);\
 MVK3OO4CO4OH + HO2 = OH + CO2 + HO2 + MGLY : 2.26e-12*exp(1300/T);\
**//Daytime Hydroxynitrates\
 ISOP1OH2N + OH = ISOP1OH2N3R4OH: 0.75*8.4e-12*exp(390/T);\
 ISOP1OH2N3R4OH + O2 = ISOP1OH2N3OO4OH: 1e-14;\
 ISOP1OH2N3R4OH = ISOP1OH23O4OH: 1.3e4*0.67;\
 ISOP1OH2N3R4OH = ISOP1OH23O4OHc: 1.3e4*.33;\
 ISOP1OH2N + OH = ISOP1OH2N3OH4OO: 0.25*8.4e-12*exp(390/T);\
 ISOP1OH2N3OH4OO + NO = ISOP1OH2N3OH4N: k_nitrate[2.7,350,2.849,11];\
 ISOP1OH2N3OH4OO + NO = MACR2N3OH + HO2 + HCHO + NO2: k_alkoxy[2.7,350,2.849,11];\
 ISOP1OH2N3OO4OH + NO = ISOP1OH2N3N4OH: k_nitrate[2.7,350,16.019,11];\
 ISOP1OH2N3OO4OH + NO = GLYC + NO2 + NO2 + HAC: k_alkoxy[2.7,350,16.019,11];\
 ISOP1OH2N3OO4OH = ISOP1CO2N3OOH4OH + HO2 : 3.75e13*exp(-10000/T);\
 ISOP1OH2N3OH4OO = ISOP1CO2N3OH4OOH + HO2 : 3.75e12*exp(-10000/T);\
 ISOP1OH2N3OH4OO + HO2 = ISOP1OH2N3OH4OOH: 2.6e-13*exp(1300/T);\
 ISOP1OH2N3OO4OH + HO2 = ISOP1OH2N3OOH4OH: 0.15*2.6e-13*exp(1300/T);\
 ISOP1OH2N3OO4OH + HO2 = GLYC + HAC + OH + NO2: 0.85*2.6e-13*exp(1300/T);\
 ISOP3N4OH + OH = ISOP1OH2R3N4OH: 0.9*1.17e-11*exp(390/T);\
 ISOP1OH2R3N4OH + O2 = ISOP1OH2OO3N4OH: 1e-14;\
 ISOP1OH2R3N4OH = ISOP1OH23O4OH: 0.67*8.42e3;\
 ISOP1OH2R3N4OH = ISOP1OH23O4OHc: 0.33*8.42e3;\
 ISOP3N4OH + OH = ISOP1OO2OH3N4OH: 0.1*1.17e-11*exp(390/T);\
 ISOP1OH2OO3N4OH + NO = MVK3N4OH + HO2 + NO2 + HCHO: 0.76*2.7E-12*exp(350/T);\
 ISOP1OH2OO3N4OH + NO = ISOP1OH2N3N4OH: k_nitrate[2.7,350,10.532,11];\
 ISOP1OH2OO3N4OH + NO = GLYC + NO2 + NO2 + HAC: k_alkoxy[2.7,350,10.532,11];\
 ISOP1OO2OH3N4OH + NO = ISOP1N2OH3N4OH: k_nitrate[2.7,350,2.849,11];\
 ISOP1OO2OH3N4OH + NO = MVK3N4OH + HO2 + NO2 + HCHO: k_alkoxy[2.7,350,2.849,11];\
 ISOP1OO2OH3N4OH = ISOP1OOH2OH3N4CO + HO2: 3.75e12*exp(-10000/T);\
 ISOP1OH2OO3N4OH = ISOP1OH2OOH3N4CO + HO2: 3.75e13*exp(-10000/T);\
 ISOP1OH2OO3N4OH + HO2 = MVK3N4OH + HO2 + OH + O2 + HCHO: 0.74*2.6e-13*exp(1300/T);\
 ISOP1OH2OO3N4OH + HO2 = ISOP1OH2OOH3N4OH: 0.15*2.6e-13*exp(1300/T);\
 ISOP1OH2OO3N4OH + HO2 = GLYC + HAC + OH + NO2: 0.11*2.6e-13*exp(1300/T);\
 ISOP1OO2OH3N4OH + HO2 = ISOP1OOH2OH3N4OH: 2.6e-13*exp(1300/T);\
**//Ozonolysis\
 ISOP + O3 = MACR + ciCH2OO : 1.1e-14*exp(-2000/T)*(0.41);\
 ISOP + O3 = MVK + ciCH2OO : 1.1e-14*exp(-2000/T)*(0.17);\
 ISOP + O3 = OH : 1.1e-14*exp(-2000/T)*(0.28);\
 ISOP + O3 = ciMVKOO : 1.1e-14*exp(-2000/T)*(0.007);\
 ISOP + O3 = ciMACROO : 1.1e-14*exp(-2000/T)*(0.006);\
 ISOP + O3 = HO2 : 1.1e-14*exp(-2000/T)*(0.16);\
 ISOP + O3 = HCHO + CO2 + HCHO + CO + CH3OO : 1.1e-14*exp(-2000/T)*0.407;****

//Reactions of SCI\

ciCH2OO + SO2 = H2SO4 : 2e-11;\
 ciCH2OO + HCOOH = HPMF : 5.6e-11;\
 ciCH2OO + H2O = HMHP : 0.9e-15*(0.73);\
 ciCH2OO + H2O = HCOOH : 0.9e-15*(0.21);\
 ciCH2OO + H2O = HCHO : 0.9e-15*(0.06);\
 ciCH2OO + H2O = H2O2 : 0.9e-15*(0.06);\
 ciCH2OO + H2Od = HMHP : 0.8e-12*(0.4);\
 ciCH2OO + H2Od = HCOOH : 0.8e-12*(0.54);\
 ciCH2OO + H2Od = HCHO : 0.8e-12*(0.06);\
 ciCH2OO + H2Od = H2O2 : 0.8e-12*(0.06);\
 ciCH2OO + O3 = HCHO : 1.0e-12*(0.7);\
 ciMACROO + H2O = MACR3OH3OOH : 1e-15;\
 ciMVKOO + H2O = MVK3OH3OOH : 1e-15;\
 HMHP + OH = HCHO + HO2 : 4.3e-12*exp(190/T)*0.5;\
 HMHP + OH = HCOOH + OH : 4.3e-12*exp(190/T)*0.5;\
 HPMF + OH = HO2 + FAH : 4.31e-12;\
 FAH + OH = CO + HO2 + CO2 : 1.80e-13;\

//NO3 Oxidation of Isoprene\

//Isoprene + NO3\

ISOP + NO3 = ISOP1N2OO : 2.95E-12*exp(-450/T)*0.42;\
 ISOP + NO3 = ISOP3OO4N : 2.95E-12*exp(-450/T)*0.045;\
 ISOP + NO3 = ISOP1N4OO : 2.95E-12*exp(-450/T)*0.45;\
 ISOP + NO3 = ISOP1OO4N : 2.95E-12*exp(-450/T)*0.085;\

//RO2 + HO2\

ISOP1N2OO + HO2 = ISOP1N2OOH : 2.47e-13*exp(1300/T)*0.47;\
 ISOP1N2OO + HO2 = MVK + OH + HCHO + NO2 : 2.47e-13*exp(1300/T)*0.53;\
 ISOP1N4OO + HO2 = ISOP1N4OOH : 2.47e-13*exp(1300/T);\
 ISOP3OO4N + HO2 = ISOP3OOH4N : 2.47e-13*exp(1300/T)*0.735;\
 ISOP3OO4N + HO2 = MACR + OH + HCHO + NO2 : 2.47e-13*exp(1300/T)*0.265;\
 ISOP1OO4N + HO2 = ISOP1OOH4N : 2.47e-13*exp(1300/T);\

//RO2 + Dominant RO2\

ISOP1N2OO + ISOP1N2OO = MVK + HCHO + NO2 + MVK + HCHO + NO2 : 6.92e-14*0.965;\
 ISOP1N2OO + ISOP1N2OO = ISOP1N2OOISOP1N2 : 6.92e-14*0.035;\
 ISOP1N2OO + ISOP3OO4N = ISOP1N2OH + ISOP3CO4N : 3.08e-12*0.77*0.5 ;\
 ISOP1N2OO + ISOP3OO4N = MVK + MACR + HCHO + HCHO + NO2 + NO2 : 3.08e-12*0.58 ;\
 ISOP1N2OO + ISOP3OO4N = ISOP3OO4NISOP1N2 : 3.08e-12*0.035 ;\
 ISOP1N2OO + ISOP1OO4N = ISOP1N2OH + ISOP1CO4N : 2.49e-12*0.77*0.5 ;\
 ISOP1N2OO + ISOP1OO4N = MVK + HCHO + NO2 + ISOP1O4N : 2.49e-12*0.58 ;\
 ISOP1N2OO + ISOP1OO4N = ISOP1OO4NISOP1N2 : 2.49e-12*0.035 ;\
 ISOP1N2OO + ISOP1N4OO = ISOP1N4CO + ISOP1N2OH : 2.49E-12*0.77*0.5;\
 ISOP1N2OO + ISOP1N4OO = MVK + HCHO + NO2 + ISOP1N4O : 2.49E-12*0.58;\
 ISOP1N2OO + ISOP1N4OO = ISOP1N2OOISOP1N4 : 2.49E-12*0.035;\
 ISOP1N4OO + ISOP1N4OO = ISOP1N4CO + ISOP1N4OHc : 3.9E-12*0.77*0.5;\
 ISOP1N4OO + ISOP1N4OO = ISOP1N4CO + ISOP1N4OHt : 3.9E-12*0.77*0.5;\
 ISOP1N4OO + ISOP1N4OO = ISOP1N4O + ISOP1N4O : 3.9E-12*0.195;\
 ISOP1N4OO + ISOP1N4OO = ISOP1N4OOISOP1N4 : 3.9E-12*0.035;\
 ISOP3OO4N + ISOP1N4OO = ISOP3OH4N + ISOP1N4CO : 3.94E-12*0.77*0.5;\
 ISOP3OO4N + ISOP1N4OO = ISOP3CO4N + ISOP1N4OHc : 3.94E-12*0.77*0.5*0.5;\
 ISOP3OO4N + ISOP1N4OO = ISOP3CO4N + ISOP1N4OHt : 3.94E-12*0.77*0.5*0.5;\
 ISOP3OO4N + ISOP1N4OO = MACR + HCHO + NO2 + ISOP1N4O : 3.94E-12*0.195;\
 ISOP3OO4N + ISOP1N4OO = ISOP3OO4NISOP1N4 : 3.94E-12*0.035;\
 ISOP1OO4N + ISOP1N4OO = ISOP1CO4N + ISOP1N4OHc : 3.29E-12*0.77*0.5*0.5;\
 ISOP1OO4N + ISOP1N4OO = ISOP1CO4N + ISOP1N4OHt : 3.29E-12*0.77*0.5*0.5;\
 ISOP1OO4N + ISOP1N4OO = ISOP1OH4Nc + ISOP1N4CO : 3.29E-12*0.77*0.5*0.5;\
 ISOP1OO4N + ISOP1N4OO = ISOP1OH4Nt + ISOP1N4CO : 3.29E-12*0.77*0.5*0.5;\
 ISOP1OO4N + ISOP1N4OO = ISOP1O4N + ISOP1N4O : 3.29E-12*0.195;\
 ISOP1OO4N + ISOP1N4OO = ISOP1OO4NISOP1N4 : 3.29E-12*0.035;\
 ISOP1N2OO + CH3OO = HCHO + ISOP1N2OH : 1.6E-13*0.71*0.5;\
 ISOP1N2OO + CH3OO = MVK + HCHO + NO2 + CH3O : 1.6E-13*0.645;\
 ISOP1N4OO + CH3OO = ISOP1N4CO + CH3OH : 1.2E-12*0.71*0.5;\
 ISOP1N4OO + CH3OO = ISOP1N4OHc + HCHO : 1.2E-12*0.71*0.5*0.5;\
 ISOP1N4OO + CH3OO = ISOP1N4OHt + HCHO : 1.2E-12*0.71*0.5*0.5;\
 ISOP1N4OO + CH3OO = ISOP1N4O + CH3O : 1.2E-12*0.29;\
 ISOP3OO4N + CH3OO = ISOP3OH4N + HCHO : 1.4E-12*0.71*0.5;\
 ISOP3OO4N + CH3OO = ISOP3CO4N + CH3OH : 1.4E-12*0.71*0.5;\
 ISOP3OO4N + CH3OO = MACR + HCHO + NO2 + CH3O : 1.4E-12*0.29;\
 ISOP1OO4N + CH3OO = ISOP1CO4N + CH3OH : 9.8E-13*0.71*0.5;\
 ISOP1OO4N + CH3OO = ISOP1OH4Nc + HCHO : 9.8E-13*0.71*0.5*0.5;\
 ISOP1OO4N + CH3OO = ISOP1OH4Nt + HCHO : 9.8E-13*0.71*0.5*0.5;\
 ISOP1OO4N + CH3OO = ISOP1O4N + CH3O : 9.8E-13*0.29;\

//RO2 + NO\

ISOP1N2OO + NO = MVK + HCHO + NO2 + NO2 : k_alkoxy[2.7,350,8.667,9];\

ISOP1N2O0 + NO = ISOP1N2N : k_nitrate[2.7,350,8.667,9];\
 ISOP1N4O0 + NO = ISOP1N4O + NO2 : k_alkoxy[2.7,350,2.319,9];\
 ISOP1N4O0 + NO = ISOP1N4N : k_nitrate[2.7,350,2.319,9];\
 ISOP3OO4N + NO = MACR + HCHO + NO2 + NO2 : k_alkoxy[2.7,350,13.202,9];\
 ISOP3OO4N + NO = ISOP3N4N : k_nitrate[2.7,350,13.202,9];\
 ISOP1OO4N + NO = ISOP1O4N + NO2 : k_alkoxy[2.7,350,2.319,9];\
 ISOP1OO4N + NO = ISOP1N4N : k_nitrate[2.7,350,2.319,9];\
 ISOP1N4O + O2 = ISOP1N4CO + HO2 : 2.5E-14*exp(-300/T);\
 ISOP1O4N + O2 = ISOP1CO4N + HO2 : 2.5E-14*exp(-300/T);\
//RO2 + NO3
 ISOP1N2O0 + NO3 = MVK + HCHO + NO2 + NO2 : 2.3E-12;\
 ISOP1N4O0 + NO3 = ISOP1N4O + NO2 : 2.3E-12;\
 ISOP3OO4N + NO3 = MACR + HCHO + NO2 + NO2 : 2.3E-12;\
 ISOP1OO4N + NO3 = ISOP1O4N + NO2 : 2.3E-12;\
//1,5 H-shift
 ISOP1N4O = ISOP1N25_3OO4OH : 1e20*exp(-10000/T);\
 ISOP1N25_3OO4OH + NO3 = ISOP1N25_3O4OH + NO2 : 2.3E-12;\
 ISOP1N25_3OO4OH + NO = ISOP1N25_3O4OH + NO2 : k_alkoxy[2.7,350,1.368,10];\
 ISOP1N25_3OO4OH + NO = ISOP1N25_3N4OH + NO2 : k_nitrate[2.7,350,1.368,10];\
 ISOP1N25_3O4OH + O2 = MACR3N + HCHO + HO2 : 2.5E-14*exp(-300/T);\
 ISOP1N25_3OO4OH + HO2 = ISOP1N25_3OOH4OH : 2.54e-13*exp(1300/T);\
 ISOP1N25_3OO4OH + ISOP1N4OO = ISOP1N25_3CO4OH + ISOP1N4OHC : 3.94E-12*0.77*0.5*0.5;\
 ISOP1N25_3OO4OH + ISOP1N4OO = ISOP1N25_3CO4OH + ISOP1N4OHC : 3.94E-12*0.77*0.5*0.5;\
 ISOP1N25_3OO4OH + ISOP1N4OO = ISOP1N25_3OH4OH + ISOP1N4CO : 3.94E-12*0.77*0.5;\
 ISOP1N25_3OO4OH + ISOP1N4OO = ISOP1N25_3O4OH + ISOP1N4O : 3.94E-12*0.195;\
 ISOP1N25_3OO4OH + ISOP1N4OO = ISOP1N25_3OO4OHISOP1N4 : 3.94E-12*0.035;\
 ISOP1N25_3OO4OH + ISOP1N2OO = MVK + HCHO + NO2 + ISOP1N25_3O4OH : 3.08e-12*0.58;\
 ISOP1N25_3OO4OH + ISOP1N2OO = ISOP1N2OH + ISOP1N25_3CO4OH : 3.08e-12*0.77*0.5;\
 ISOP1N25_3OO4OH + ISOP1N2OO = ISOP1N25_3OO4OHISOP1N2 : 3.08e-12*0.035;\
 ISOP1N25_3OO4OH + CH3OO = ISOP1N25_3OH4OH + HCHO : 1.4E-12*0.71*0.5;\
 ISOP1N25_3OO4OH + CH3OO = ISOP1N25_3CO4OH + CH3OH : 1.4E-12*0.71*0.5;\
 ISOP1N25_3OO4OH + CH3OO = ISOP1N25_3O4OH + CH3O : 1.4E-12*0.29;\
//NPN
 ISOP1N2OOH + OH = ISOP1N2OOH3R4OH : 8.38e-12*exp(390/T)*0.76;\
 ISOP1N2OOH3R4OH + O2 = ISOP1N2OOH3OO4OH : 1e-14;\
 ISOP1N2OOH3R4OH = ISOP1N2O4OH + OH : 9.2e4;\
 ISOP1N2OOH + OH = ISOP1N2OOH3OH4OO : 8.38e-12*exp(390/T)*0.24;\
 ISOP1N4OOH + OH = ISOP1N2OH3R4OOH : 2.24e-11*exp(390/T)*0.31;\
 ISOP1N2OH3R4OOH + O2 = ISOP1N2OH3OO4OOH : 1e-14;\
 ISOP1N2OH3R4OOH = ISOP1N2OH34O + OH : 9.61e4;\
 ISOP1N4OOH + OH = ISOP1N2R3OH4OOH : 2.24e-11*exp(390/T)*0.69;\
 ISOP1N2R3OH4OOH + O2 = ISOP1N2OO3OH4OOH : 1e-14;\
 ISOP1N2R3OH4OOH = ISOP12O3OH4OOH + NO2 : 7.73e3;\
 ISOP3OOH4N + OH = ISOP1OH2R3OOH4N : 1.17e-11*exp(390/T)*0.965;\
 ISOP1OH2R3OOH4N + O2 = ISOP1OH2OO3OOH4N : 1e-14;\
 ISOP1OH2R3OOH4N = ISOP1OH23O4N + OH : 9.2e4;\
 ISOP3OOH4N + OH = ISOP1OO2OH3OOH4N : 1.17e-11*exp(390/T)*0.035;\
 ISOP1OOH4N + OH = ISOP1OOH2R3OH4N : 3.07e-11*exp(390/T)*0.69;\
 ISOP1OOH2R3OH4N + O2 = ISOP1OOH2OO3OH4N : 1e-14;\
 ISOP1OOH2R3OH4N = ISOP12O3OH4N + OH : 9.61e4;\
 ISOP1OOH4N + OH = ISOP1OOH2OH3R4N : 3.07e-11*exp(390/T)*0.31;\
 ISOP1OOH2OH3R4N + O2 = ISOP1OOH2OH3OO4N : 1e-14;\
 ISOP1OOH2OH3R4N = ISOP1OOH2OH34O + NO2 : 7.73e3;\
 ISOP1N2OOH + OH = ISOP1N2OO + H2O : 3.4E-12*exp(200/T);\
 ISOP1N4OOH + OH = ISOP1N4OO + H2O : 3.4E-12*exp(200/T);\
 ISOP3OOH4N + OH = ISOP3OO4N + H2O : 3.4E-12*exp(200/T);\
 ISOP1OOH4N + OH = ISOP1OO4N + H2O : 3.4E-12*exp(200/T);\
//ISOPNOOHOHO
 ISOP1N2OOH3OO4OH + NO = ISOP1N2OOH3N4OH : k_nitrate[2.7,350,3.322,12];\
 ISOP1N2OOH3OO4OH + NO = NO2 + PROPNN + GLYC + OH : k_alkoxy[2.1375,350,3.322,12];\
 ISOP1N2OOH3OO4OH + NO = NO2 + HO2 + HCHO + MACR2OOH3N : k_alkoxy[0.5625,350,3.322,12];\
 ISOP1N2OOH3OO4OH + HO2 = NO2 + HO2 + HCHO + MACR2OOH3N : 0.15*2.64e-13*exp(1300/T);\
 ISOP1N2OOH3OO4OH + HO2 = OH + PROPNN + GLYC + OH : 0.58*2.64e-13*exp(1300/T);\
 ISOP1N2OOH3OO4OH + HO2 = ISOP1N2OOH3OOH4OH : 0.27*2.64e-13*exp(1300/T);\
 ISOP1N2OOH3OH4OO + NO = ISOP1N2OOH3OH4N : k_nitrate[2.7,350,2.567,12];\
 ISOP1N2OOH3OH4OO + NO = NO2 + HO2 + HCHO + MACR2OOH3N : k_alkoxy[2.7,350,2.567,12];\
 ISOP1N2OOH3OH4OO + HO2 = ISOP1N2OOH3OH4OOH : 2.64e-13*exp(1300/T);\
 ISOP1N2OH3OO4OOH + NO = ISOP1N2OH3N4OOH : k_nitrate[2.7,350,3.322,12];\
 ISOP1N2OH3OO4OOH + NO = NO2 + MACR2OH3N + HCHO + OH : k_alkoxy[0.5625,350,3.322,12];\
 ISOP1N2OH3OO4OOH + NO = NO2 + PROPNN + HPETHNL + HO2 : k_alkoxy[2.1375,350,3.322,12];\
 ISOP1N2OH3OO4OOH + HO2 = OH + PROPNN + HPETHNL + HO2 : 0.58*2.64e-13*exp(1300/T);\
 ISOP1N2OH3OO4OOH + HO2 = OH + MACR2OH3N + HCHO + OH : 0.15*2.64e-13*exp(1300/T);\
 ISOP1N2OH3OO4OOH + HO2 = ISOP1N2OH3OOH4OOH : 0.27*2.64e-13*exp(1300/T);

ISOP1N2O03OH4OOH + NO = ISOP1N2N3OH4OOH : k_nitrate[2.7,350,9.617,12];\
 ISOP1N2O03OH4OOH + NO = NO2 + PROPNN + HPETHNL + HO2 : k_alkoxy[2.7,350,9.617,12];\
 ISOP1N2O03OH4OOH + HO2 = OH + PROPNN + HPETHNL + HO2 : 0.73*2.64e-13*exp(1300/T);\
 ISOP1N2O03OH4OOH + HO2 = ISOP1N2OOH3OH4OOH : 0.27*2.64e-13*exp(1300/T);\
 ISOP1OH2O03OOH4N + NO = ISOP1OH2N3OOH4N : k_nitrate[2.7,350,2.063,12];\
 ISOP1OH2O03OOH4N + NO = NO2 + HO2 + HCHO + MVK3OOH4N : k_alkoxy[0.5625,350,2.063,12];\
 ISOP1OH2O03OOH4N + NO = NO2 + HAC + ETHLN + OH : k_alkoxy[2.1375,350,2.063,12];\
 ISOP1OH2O03OOH4N + HO2 = OH + HAC + ETHLN + OH : 0.58*2.64e-13*exp(1300/T);\
 ISOP1OH2O03OOH4N + HO2 = OH + HO2 + HCHO + MVK3OOH4N : 0.15*2.64e-13*exp(1300/T);\
 ISOP1OH2O03OOH4N + HO2 = ISOP1OH2OOH3OOH4N : 0.27*2.64e-13*exp(1300/T);\
 ISOP1OO2OH3OOH4N + NO = ISOP1N2OH3OOH4N : k_nitrate[2.7,350,2.567,12];\
 ISOP1OO2OH3OOH4N + NO = HO2 + HO2 + HCHO + MVK3OOH4N : k_alkoxy[2.7,350,2.567,12];\
 ISOP1OO2OH3OOH4N + HO2 = ISOP1OOH2OH3OOH4N : 2.64e-13*exp(1300/T);\
 ISOP1OOH2O03OH4N + NO = ISOP1OOH2N3OH4N : k_nitrate[2.7,350,2.063,12];\
 ISOP1OOH2O03OH4N + NO = NO2 + HPAC + ETHLN + HO2 : k_alkoxy[2.1375,350,2.063,12];\
 ISOP1OOH2O03OH4N + NO = NO2 + MVK3OH4N + HCHO + OH : k_alkoxy[0.5625,350,2.063,12];\
 ISOP1OOH2O03OH4N + HO2 = OH + MVK3OH4N + HCHO + OH : 0.15*2.64e-13*exp(1300/T);\
 ISOP1OOH2O03OH4N + HO2 = OH + HPAC + ETHLN + HO2 : 0.58*2.64e-13*exp(1300/T);\
 ISOP1OOH2O03OH4N + HO2 = ISOP1OOH2OOH3OH4N : 0.27*2.64e-13*exp(1300/T);\
 ISOP1OOH2OH3OO4N + NO = ISOP1OOH2OH3N4N : k_nitrate[2.7,350,14.652,12];\
 ISOP1OOH2OH3OO4N + NO = NO2 + HPAC + ETHLN + HO2 : k_alkoxy[2.7,350,14.652,12];\
 ISOP1OOH2OH3OO4N + HO2 = OH + HPAC + ETHLN + HO2 : 0.73*2.64e-13*exp(1300/T);\
 ISOP1OOH2OH3OO4N + HO2 = ISOP1OOH2OH3OOH4N : 0.27*2.64e-13*exp(1300/T);\
 ISOP1N2OOH3OO4OH = ISOP1N2OO3OOH4OH : 4e6;\
 ISOP1N2OOH3OH4OO = ISOP1N2OO3OH4OOH : 4e6;\
 ISOP1N2OH3OO4OOH = ISOP1N2OH3OOH4OO : 2e6;\
 ISOP1N2OO3OH4OOH = ISOP1N2OOH3OH4OO : 2e6;\
 ISOP1OH2O03OOH4N = ISOP1OH2OOH3OO4N : 3e6;\
 ISOP1OO2OH3OOH4N = ISOP1OOH2OH3OO4N : 3e6;\
 ISOP1OOH2O03OH4N = ISOP1OO2OOH3OH4N : 2e6;\
 ISOP1OOH2OH3OO4N = ISOP1OO2OH3OOH4N : 2e6;\
 ISOP1N2OO3OOH4OH = ISOP1N2OOH3OO4OH : 3e6;\
 ISOP1N2OH3OOH4OO = ISOP1N2OH3OO4OOH : 3e6;\
 ISOP1OH2OOH3OO4N = ISOP1OH2OO3OOH4N : 4e6;\
 ISOP1OO2OOH3OH4N = ISOP1OOH2OO3OH4N : 4e6;\
 ISOP1N2OO3OOH4OH + HO2 = ISOP1N2OOH3OOH4OH : 0.27*2.64e-13*exp(1300/T);\
 ISOP1N2OO3OOH4OH + HO2 = MVK3OOH4OH + NO2 + CH2O + OH : 0.15*2.64e-13*exp(1300/T);\
 ISOP1N2OO3OOH4OH + HO2 = OH + OH + GLYC + PROPNN : 0.58*2.64e-13*exp(1300/T);\
 ISOP1N2OO3OOH4OH + NO = ISOP1N2N3OOH4OH : k_nitrate[2.7,350,17.17,12];\
 ISOP1N2OO3OOH4OH + NO = MVK3OOH4OH + NO2 + CH2O : k_alkoxy[0.5625,350,17.17,12];\
 ISOP1N2OO3OOH4OH + NO = NO2 + OH + GLYC + PROPNN : k_alkoxy[2.1375,350,17.17,12];\
 ISOP1N2OH3OOH4OO + HO2 = ISOP1N2OH3OOH4OOH : 2.64e-13*exp(1300/T);\
 ISOP1N2OH3OOH4OO + NO = ISOP1N2OH3OOH4N : k_nitrate[2.7,350,4.833,12];\
 ISOP1N2OH3OOH4OO + NO = MACR2OH3N + OH + NO2 + CH2O : k_alkoxy[2.7,350,4.833,12];\
 ISOP1OH2OOH3OO4N + HO2 = ISOP1OH2OOH3OOH4N : 0.27*2.64e-13*exp(1300/T);\
 ISOP1OH2OOH3OO4N + HO2 = MACR2OOH3OH + OH + NO2 + CH2O : 0.15*2.64e-13*exp(1300/T);\
 ISOP1OH2OOH3OO4N + HO2 = HAC + ETHLN + OH + OH : 0.58*2.64e-13*exp(1300/T);\
 ISOP1OH2OOH3OO4N + NO = ISOP1OH2OOH3N4N : k_nitrate[2.7,350,25.983,12];\
 ISOP1OH2OOH3OO4N + NO = MACR2OOH3OH + NO2 + NO2 + CH2O : k_alkoxy[0.5625,350,25.983,12];\
 ISOP1OO2OOH3OH4N + NO = HAC + ETHLN + OH + NO2 : k_alkoxy[2.1375,350,25.983,12];\
 ISOP1OO2OOH3OH4N + HO2 = ISOP1OOH2OOH3OH4N : 2.64e-13*exp(1300/T);\
 ISOP1OO2OOH3OH4N + NO = ISOP1N2OOH3OH4N : k_nitrate[2.7,350,4.833,12];\
 ISOP1OO2OOH3OH4N + NO = MVK3OH4N + OH + NO2 + CH2O : k_alkoxy[2.7,350,4.833,12];\
 //INHE\
 ISOP1N23O4OH + OH = NO2 + ISOP1CO23O4OH : 4.78e-11*exp(-400/T)*0.69;\
 ISOP1N23O4OH + OH = ISOP1N2OO3CO4OH : 4.78e-11*exp(-400/T)*0.07;\
 ISOP1N23O4OH + OH = ISOP1N23O4OH4R : 4.78e-11*exp(-400/T)*0.24;\
 ISOP1N23O4OH4R + O2 = ISOP1N23O4CO + HO2 : 1e-14;\
 ISOP1N23O4OH4R = CH2O + NO2 + MVKENOL : 0.5*2.07e5;\
 ISOP1N23O4OH4R = ISOP1N2OH3OO4CO : 0.5*2.07e5;\
 ISOP1OH23O4N + OH = ISOP1OH23O4CO + NO2 : 4.78e-11*exp(-400/T)*0.24;\
 ISOP1OH23O4N + OH = ISOP1OH2OO3CO4N : 4.78e-11*exp(-400/T)*0.07;\
 ISOP1OH23O4N + OH = ISOP1OH1R23O4N : 4.78e-11*exp(-400/T)*0.69;\
 ISOP1OH1R23O4N + O2 = ISOP1CO23O4N + HO2 : 1e-14;\
 ISOP1OH1R23O4N = CH2O + NO2 + MCRENOL : 0.5*2.07e5;\
 ISOP1OH1R23O4N = ISOP1CO2OO3OH4N : 0.5*2.07e5;\
 ISOP1N2OH34O + OH = NO2 + ISOP1CO2OH34O : 3.22e-11*exp(-400/T);\
 ISOP12O3OH4N + OH = ISOP12O3OH4CO + NO2 : 0.2*3.22e-11*exp(-400/T);\
 ISOP12O3OH4N + OH = ISOP12O3OH3R4N : 0.8*3.22e-11*exp(-400/T);\
 ISOP12O3OH3R4N + O2 = ISOP12O3CO4N + HO2 : 0.33*1e-14;\
 ISOP12O3OH3R4N + O2 = ISOP1OH3OH4CO + NO2 : 0.67*1e-14;\
 ISOP12O3OH3R4N = ISOP1OH2OO3CO4N : 3.45e4;\
 //ICN\

ISOP3CO4N + OH = ISOP1OH2OO3CO4N : 1.17e-11*exp(390/T);\
 ISOP1OH2OO3CO4N + HO2 = ISOP1OH2OOH3CO4N : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1OH2OO3CO4N + HO2 = HAC + OH + NPA : 2.6e-13*exp(1300/T)*0.58;\
 ISOP1OH2OO3CO4N + HO2 = MVK3CO4N + HO2 + OH + CH2O : 2.6e-13*exp(1300/T)*0.15;\
 ISOP1OH2OO3CO4N + NO = MVK3CO4N + NO2 + HO2 + CH2O: k_alkoxy[0.5625,350,7.239,11];\
 ISOP1OH2OO3CO4N + NO = ISOP1OH2N3CO4N : k_nitrate[2.7,350,7.239,11];\
 ISOP1OH2OO3CO4N + NO = HAC + NO2 + NPA : k_alkoxy[2.1375,350,7.239,11];\
 ISOP1N2OO3CO4OH + NO = ISOP1N2N3CO4OH: k_nitrate[2.7,350,76.383,11];\
 ISOP1N2OO3CO4OH + NO = MVK3CO4OH + CH2O + NO2 + NO2: k_alkoxy[0.5625,350,76.383,11];\
 ISOP1N2OO3CO4OH + NO = NO2 + PROPNN + CH3CO3: k_alkoxy[2.1375,350,76.383,11];\
 ISOP1N2OO3CO4OH + HO2 = OH + PROPNN + CH3CO3 : 2.6e-13*exp(1300/T)*0.58;\
 ISOP1N2OO3CO4OH + HO2 = MVK3CO4OH + CH2O + NO2 + OH : 2.6e-13*exp(1300/T)*0.15;\
 ISOP1N2OO3CO4OH + HO2 = ISOP1N2OOH3CO4OH : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1N4CO + OH = ISOP1N4R4CO : 4.13e-12*exp(470/T);\
 ISOP1N4R4CO = NO2 + ISOP12O344CO : 1.294e4;\
 ISOP1N4R4CO + O2 = ISOP1N2OO344CO : 0.875*1e-14;\
 ISOP1N4R4CO + O2 = ISOP1N4CO4OO : 0.125*1e-14;\
 ISOP1N2OO344CO + NO = ISOP1N2N344CO : k_nitrate[2.7,350,7.948,10];\
 ISOP1N2OO344CO + NO = NO2 + NO2 + CH2O + MVK4CO : k_alkoxy[2.7,350,7.948,10];\
 ISOP1N2OO344CO + HO2 = OH + NO2 + CH2O + MVK4CO : 2.54e-13*exp(1300/T)*0.54;\
 ISOP1N2OO344CO + HO2 = ISOP1N2OOH344CO : 2.54e-13*exp(1300/T)*0.47;\
 ISOP1N4CO4OO + NO2 + M = ISOP1N4PAN + M : k_troe[k_0 = 2.133e-28*(T/300)^(-7.1), k_inf= 1.2e-11*(T/300)^(-0.9), Fc = 0.3];\
 ISOP1N4CO4OO + NO = NO2 + CO2 + C4NVP2 : 2.7E-12*exp(350/T);\
 ISOP1N4CO4OO + HO2 = ISOP1N4CO4OOH : 2.54e-13*exp(1300/T)*0.4;\
 ISOP1N4CO4OO + HO2 = O3 + ISOP1N4CO4OH : 2.54e-13*exp(1300/T)*0.2;\
 ISOP1N4CO4OO + HO2 = OH + CO2 + C4NVP2 : 2.54e-13*exp(1300/T)*0.4;\
 C4NVP2 + NO = NO2 + MACR2OO3N : 2.7E-12*exp(350/T);\
 C4NVP2 + HO2 = OH + MACR2OO3N : 2.38e-13*exp(1300/T);\
 C4NVP2 + NO2 = MACR2N3N : 9e-12;\
 MACR2OO3N + NO = NO2 + HO2 + CO + PROPNN : 2.7E-12*exp(350/T);\
 MACR2OO3N + HO2 = OH + HO2 + CO + PROPNN : 2.47e-13*exp(1300/T);\
 ISOP1N4PAN + M = ISOP1N4CO4OO + NO2 + M : k_troe[k_0 = 3.871e-3*exp(-12100/T), k_inf = 5.4e16*exp(-13830/T), Fc = 0.3];\
 ISOP1CO4N + OH = ISOP1CO1R4N : 4.13e-12*exp(470/T);\
 ISOP1CO1R4N = NO2 + ISOP121CO34O : 1.294e4;\
 ISOP1CO1R4N + O2 = ISOP121CO3OO4N : 0.875*1e-14;\
 ISOP1CO1R4N + O2 = ISOP1CO1OO4N : 0.125*1e-14;\
 ISOP121CO3OO4N + NO = ISOP121CO3N4N : k_nitrate[2.7,350,12.136,10];\
 ISOP121CO3OO4N + NO = NO2 + NO2 + CH2O + MACR3CO : k_alkoxy[2.7,350,12.136,10];\
 ISOP121CO3OO4N + HO2 = OH + NO2 + CH2O + MACR3CO : 2.54e-13*exp(1300/T)*0.26;\
 ISOP121CO3OO4N + HO2 = ISOP121CO3OOH4N : 2.54e-13*exp(1300/T)*0.74;\
 ISOP1CO1OO4N + NO2 + M = ISOP1PAN4N + M : k_troe[k_0 = 2.133e-28*(T/300)^(-7.1), k_inf= 1.2e-11*(T/300)^(-0.9), Fc = 0.3];\
 ISOP1CO1OO4N + NO = NO2 + CO2 + C4NVP1 : 2.7E-12*exp(350/T);\
 ISOP1CO1OO4N + HO2 = ISOP1CO1OOH4N : 2.54e-13*exp(1300/T)*0.4;\
 ISOP1CO1OO4N + HO2 = O3 + ISOP1CO1OH4N : 2.54e-13*exp(1300/T)*0.2;\
 ISOP1CO1OO4N + HO2 = OH + CO2 + C4NVP1 : 2.54e-13*exp(1300/T)*0.4;\
 C4NVP1 + NO = NO2 + MVK3OO4N : 2.7E-12*exp(350/T);\
 C4NVP1 + HO2 = OH + MVK3OO4N : 2.38e-13*exp(1300/T);\
 C4NVP1 + NO2 = MVK3N4N : 9e-12;\
 MVK3OO4N + NO = NO2 + ETHLN + CH3CO3 : 2.7E-12*exp(350/T);\
 MVK3OO4N + HO2 = OH + ETHLN + CH3CO3 : 2.47e-13*exp(1300/T);\
 ISOP1PAN4N + M = ISOP1N4CO4OO + NO2 + M : k_troe[k_0 = 3.871e-3*exp(-12100/T), k_inf = 5.4e16*exp(-13830/T), Fc = 0.3];\
 ISOP1N4CO + OH = ISOP1N2R3OH4CO : 2.24e-11*exp(390/T)*0.69;\
 ISOP1N2R3OH4CO + O2 = ISOP1N2OO3OH4CO : 1e-14;\
 ISOP1N2R3OH4CO = ISOP12O3OH4CO + NO2 : 7.73e3;\
 ISOP1N4CO + OH = ISOP1N2OH3OO4CO : 2.24e-11*exp(390/T)*0.31;\
 ISOP1CO4N + OH = ISOP1CO2OH3R4N : 3.07e-11*exp(390/T)*0.31;\
 ISOP1CO2OH3R4N + O2 = ISOP1CO2OH3OO4N : 1e-14;\
 ISOP1CO2OH3R4N = ISOP1CO2OH34O + NO2 : 7.73e3;\
 ISOP1CO4N + OH = ISOP1CO2OO3OH4N : 3.07e-11*exp(390/T)*0.69;\
 ISOP1N2OO3OH4CO = MACR2OOH3N + CO + HO2 : 4e8*exp(-5000/T);\
 ISOP1CO2OH3OO4N = MVK3OOH4N + CO + HO2 : 4e8*exp(-5000/T);\
 ISOP1N2OH3OO4CO = MACR2OH3N + CO + OH : 1e7*exp(-5000/T);\
 ISOP1N2OH3OO4CO + HO2 = ISOP1N2OH3OOH4CO : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1N2OH3OO4CO + HO2 = MACR2OH3N + OH + HO2 + CO : 2.6e-13*exp(1300/T)*0.15;\
 ISOP1N2OH3OO4CO + HO2 = OH + HO2 + PROPNN + GLYX : 2.6e-13*exp(1300/T)*0.58;\
 ISOP1N2OH3OO4CO + NO = ISOP1N2OH3N4CO : k_nitrate[2.7,350,16.019,11];\
 ISOP1N2OH3OO4CO + NO = MACR2OH3N + NO2 + HO2 + CO : k_alkoxy[0.5625,350,16.019,11];\
 ISOP1N2OH3OO4CO + NO = NO2 + HO2 + PROPNN + GLYX : k_alkoxy[2.1375,350,16.019,11];\
 ISOP1CO2OO3OH4N = MVK3OH4N + CO + OH : 1e7*exp(-5000/T);\
 ISOP1CO2OO3OH4N + HO2 = MVK3OH4N + OH + HO2 + CO : 2.6e-13*exp(1300/T)*0.15;\
 ISOP1CO2OO3OH4N + HO2 = OH + HO2 + MGLY + ETHLN : 2.6e-13*exp(1300/T)*0.58;\
 ISOP1CO2OO3OH4N + HO2 = ISOP1CO2OOH3OH4N : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1CO2OO3OH4N + NO = MVK3OH4N + NO2 + HO2 + CO : k_alkoxy[0.5625,350,10.532,11];\

ISOP1CO2OO3OH4N + NO = NO2 + HO2 + MGLY + ETHLN : k_alkoxy[2.1375,350,10.532,11];\
 ISOP1CO2OO3OH4N + NO = ISOP1CO2N3OH4N : k_nitrate[2.7,350,10.532,11];\
 //HHN\
 ISOP1N2OH + OH = ISOP1N2OH3OO4OH : 8.38e-12*exp(390/T)*0.76;\
 ISOP1N2OH + OH = ISOP1N2OH3OH4OO : 8.38e-12*exp(390/T)*0.24;\
 ISOP1N4OHc + OH = ISOP1N2R3OH4OH : 2.24e-11*exp(390/T)*0.69;\
 ISOP1N4OHt + OH = ISOP1N2R3OH4OH : 2.24e-11*exp(390/T)*0.69;\
 ISOP1N2R3OH4OH + O2 = ISOP1N2OO3OH4OH : 1e-14;\
 ISOP1N2R3OH4OH = ISOP1O3OH4OH : 7.73e3;\
 ISOP1N4OHc + OH = ISOP1N2OH3OO4OH : 2.24e-11*exp(390/T)*0.31;\
 ISOP1N4OHt + OH = ISOP1N2OH3OO4OH : 2.24e-11*exp(390/T)*0.31;\
 ISOP3OH4N + OH = ISOP1OH2OO3OH4N : 1.17e-11*exp(390/T)*0.965;\
 ISOP3OH4N + OH = ISOP1OO2OH3OH4N : 1.17e-11*exp(390/T)*0.035;\
 ISOP1OH4Nc + OH = ISOP1OH2OH3R4N : 3.07e-11*exp(390/T)*0.31;\
 ISOP1OH4Nt + OH = ISOP1OH2OH3R4N : 3.07e-11*exp(390/T)*0.31;\
 ISOP1OH2OH3R4N + O2 = ISOP1OH2OH3OO4N : 1e-14;\
 ISOP1OH2OH3R4N = ISOP1OH2OH34O : 7.73e3;\
 ISOP1OH4Nc + OH = ISOP1OH2OO3OH4N : 3.07e-11*exp(390/T)*0.69;\
 ISOP1OH4Nt + OH = ISOP1OH2OO3OH4N : 3.07e-11*exp(390/T)*0.69;\
 ISOP1N2OO3OH4OH + HO2 = ISOP1N2OOH3OH4OH : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1N2OO3OH4OH + HO2 = OH + HO2 + PROPNN + GLYC : 2.6e-13*exp(1300/T)*0.73;\
 ISOP1N2OH3OO4OH + HO2 = ISOP1N2OH3OOH4OH : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1N2OH3OO4OH + HO2 = MACR2OH3N + HCHO + HO2 + OH : 2.6e-13*exp(1300/T)*0.73*0.21;\
 ISOP1N2OH3OO4OH + HO2 = OH + HO2 + PROPNN + GLYC : 2.6e-13*exp(1300/T)*0.73*0.79;\
 ISOP1OH2OH3OO4N + HO2 = ISOP1OH2OH3OOH4N : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1OH2OH3OO4N + HO2 = OH + HO2 + HAC + ETHLN : 2.6e-13*exp(1300/T)*0.73;\
 ISOP1OH2OO3OH4N + HO2 = ISOP1OH2OOH3OH4N : 2.6e-13*exp(1300/T)*0.27;\
 ISOP1OH2OO3OH4N + HO2 = MVK3OH4N + HCHO + HO2 + OH : 2.6e-13*exp(1300/T)*0.73*0.21;\
 ISOP1OH2OO3OH4N + HO2 = OH + HO2 + HAC + ETHLN : 2.6e-13*exp(1300/T)*0.73*0.79;\
 ISOP1N2OO3OH4OH + NO = ISOP1N2N3OH4OH : k_nitrate[2.7,350,10.532,11];\
 ISOP1N2OO3OH4OH + NO = NO2 + HO2 + PROPNN + GLYC : k_alkoxy[2.7,350,10.532,11];\
 ISOP1N2OH3OO4OH + NO = ISOP1N2OH3N4OH : k_nitrate[2.7,350,1.908,11];\
 ISOP1N2OH3OO4OH + NO = MACR2OH3N + HCHO + HO2 + NO2 : k_alkoxy[0.567,350,1.908,11];\
 ISOP1N2OH3OO4OH + NO = NO2 + HO2 + PROPNN + GLYC : k_alkoxy[2.133,350,1.908,11];\
 ISOP1OH2OH3OO4N + NO = ISOP1OH2OH3N4N : k_nitrate[2.7,350,16.019,11];\
 ISOP1OH2OH3OO4N + NO = NO2 + HO2 + HAC + ETHLN : k_alkoxy[2.7,350,16.019,11];\
 ISOP1OH2OO3OH4N + NO = ISOP1OH2N3OH4N : k_nitrate[2.7,350,1.124,11];\
 ISOP1OH2OO3OH4N + NO = MVK3OH4N + HCHO + HO2 + NO2 : k_alkoxy[0.567,350,1.124,11];\
 ISOP1OH2OO3OH4N + NO = NO2 + HO2 + HAC + ETHLN : k_alkoxy[2.133,350,1.124,11];\
 ISOP1N2OH3OH4OO + HO2 = ISOP1N2OH3OH4OOH : 2.6e-13*exp(1300/T);\
 ISOP1OO2OH3OH4N + HO2 = ISOP1OOH2OH3OH4N : 2.6e-13*exp(1300/T);\
 ISOP1N2OH3OH4OO + NO = ISOP1N2OH3OH4N : k_nitrate[2.7,350,2.849,11];\
 ISOP1N2OH3OH4OO + NO = HO2 + NO2 + CH2O + MACR2OH3N : k_alkoxy[2.7,350,2.849,11];\
 ISOP1OO2OH3OH4N + NO = ISOP1N2OH3OH4N : k_nitrate[2.7,350,2.849,11];\
 ISOP1OO2OH3OH4N + NO = HO2 + NO2 + CH2O + MVK3OH4N : k_alkoxy[2.7,350,2.849,11];

Table I.4: Alternate formulations of epoxide formation reactions for the explicit isoprene mechanism. These reactions replace the italicized reactions found in Table I.3.

ISOP1OH2OOH + OH = ISOP1OH2OOH3OO4OH : 1.7e-11*exp(390/T)*0.95*0.10;\n
 ISOP1OH2OOH + OH = ISOP1OH23O4OHt : 1.7e-11*exp(390/T)*0.95*0.67*[1/(4.77e-21*[M]+1)];\n
 ISOP1OH2OOH + OH = ISOP1OH23O4OHc : 1.7e-11*exp(390/T)*0.95*0.33*[1/(4.77e-21*[M]+1)];\n
 ISOP3OOH4OH + OH = ISOP1OH2OO3OOH4OH : 3.0e-11*exp(390/T)*0.95*0.10;\n
 ISOP3OOH4OH + OH = ISOP1OH23O4OHt : 3.0e-11*exp(390/T)*0.95*0.68*[1/(4.77e-21*[M]+1)];\n
 ISOP3OOH4OH + OH = ISOP1OH23O4OHc : 3.0e-11*exp(390/T)*0.95*0.32*[1/(4.77e-21*[M]+1)];\n
 ISOP1OH23O4OHc + OH = ISOP1OH23O4CO + H2O + HO2 : 0.168*0.228*5.82e-11*exp(-400/T);\n
 ISOP1OH23O4OHc + OH = HAC + GLYX + OH : 0.168*0.63*5.82e-11*exp(-400/T)*[1/(1.20e-20*[M]+1)];\n
 ISOP1OH23O4OHc + OH = MACR2OH3OH + OH + CO : 0.168*0.37*5.82e-11*exp(-400/T)*[1/(1.20e-20*[M]+1)];\n
 ISOP1OH23O4OHc + OH = ISOP1CO23O4OH + H2O + HO2 : 0.752*0.228*5.82e-11*exp(-400/T);\n
 ISOP1OH23O4OHc + OH = GLYC + MGLY + OH : 0.752*0.287*5.82e-11*exp(-400/T)*[1/(1.20e-20*[M]+1)];\n
 ISOP1OH23O4OHc + OH = MVK3OH4OH + OH + CO : 0.752*0.713*5.82e-11*exp(-400/T)*[1/(1.20e-20*[M]+1)];\n
 ISOP1OH23O4OHt + OH = ISOP1OH23O4CO + H2O + HO2 : 0.31*0.194*3.75e-11*exp(-400/T);\n
 ISOP1OH23O4OHt + OH = HAC + GLYX + OH : 0.31*0.63*3.75e-11*exp(-400/T)*[1/(9.77e-21*[M]+1)];\n
 ISOP1OH23O4OHt + OH = MACR2OH3OH + OH + CO : 0.31*0.37*3.75e-11*exp(-400/T)*[1/(9.77e-21*[M]+1)];\n
 ISOP1OH23O4OHt + OH = ISOP1CO23O4OH + H2O + HO2 : 0.62*0.194*3.75e-11*exp(-400/T);\n
 ISOP1OH23O4OHt + OH = GLYC + MGLY + OH : 0.62*0.287*3.75e-11*exp(-400/T)*[1/(9.77e-21*[M]+1)];\n
 ISOP1OH23O4OHt + OH = MVK3OH4OH + OH + CO : 0.62*0.713*3.75e-11*exp(-400/T)*[1/(9.77e-21*[M]+1)];\n
 ISOP12O3OH4OH + OH = ISOP12O3CO4OH + HO2 : 0.8*0.2*3.22e-11*exp(-400/T);\n
 ISOP12O3OH4OH + OH = ISOP1OH3OH4CO + HO2 : 0.8*0.4*3.22e-11*exp(-400/T);\n
 ISOP12O3OH4OH + OH = ISOP1OH2OO3CO4OH : 0.8*3.22e-11*exp(-400/T)*[1/(6.09e-20*[M]+1)];\n
 ISOP1CO4OOHc + OH = ISOP1CO2OH3OO4OOH : 5.0e-13*exp(650/T);\n
 ISOP1CO4OOHc + OH = ISOP1CO2OH34O : 1.0e-12*exp(650/T)*[1/(4.058e-20*[M]+1)];\n
 ISOP1CO4OOHc + OH = ISOP1CO1OOH4CO : 3.8e-12*exp(400/T)*0.1;\n
 ISOP1CO4OOHc + OH = ISOP121CO3OO4OOH : 3.8e-12*exp(400/T)*0.7;\n
 ISOP1CO4OOHc + OH = ISOP121CO34O : 3.8e-12*exp(400/T)*[1/(1.623e-19*[M]+1)];\n
 ISOP1CO4OOc = ISOP1CO1OOH4CO : 10*0.1;\n
 ISOP1CO4OOc = ISOP121CO3OO4OOH : 10*0.7;\n
 ISOP1CO4OOc = ISOP121CO34O : 10*[1/(1.623e-19*[M]+1)];\n
 ISOP1OOH4COc + OH = ISOP1OOH2OO3OH4CO : 1.0e-12*exp(650/T);\n
 ISOP1OOH4COc + OH = ISOP12O3OH4CO : 2.0e-12*exp(650/T)*[1/(4.058e-20*[M]+1)];\n
 ISOP1OOH4COc + OH = ISOP1OOH2OO344CO : 3.8e-12*exp(400/T)*0.7;\n
 ISOP1OOH4COc + OH = ISOP1CO4CO4OOH : 3.8e-12*exp(400/T)*0.1;\n
 ISOP1OOH4COc + OH = ISOP12O344CO : 3.8e-12*exp(400/T)*[1/(1.623e-19*[M]+1)];\n
 ISOP1OO4COc = ISOP1OOH2OO344CO : 10*0.7;\n
 ISOP1OO4COc = ISOP1CO4CO4OOH : 10*0.1;\n
 ISOP1OO4COc = ISOP12O344CO : 10*[1/(1.623e-19*[M]+1)];\n
 ISOP1OH2N + OH = ISOP1OH2N3OO4OH : 0.75*0.8*8.4e-12*exp(390/T);\n
 ISOP1OH2N + OH = ISOP1OH23O4OHt : 0.75*0.67*8.4e-12*exp(390/T)*[1/(1.62e-19*[M]+1)];\n
 ISOP1OH2N + OH = ISOP1OH23O4OHc : 0.75*0.33*8.4e-12*exp(390/T)*[1/(1.62e-19*[M]+1)];\n
 ISOP3N4OH + OH = ISOP1OH2OO3N4OH : 0.9*0.86*1.17e-11*exp(390/T);\n
 ISOP3N4OH + OH = ISOP1OH23O4OHt : 0.9*0.67*1.17e-11*exp(390/T)*[1/(2.49e-19*[M]+1)];\n
 ISOP3N4OH + OH = ISOP1OH23O4OHc : 0.9*0.33*1.17e-11*exp(390/T)*[1/(2.49e-19*[M]+1)];\n
 ISOP1N2OOH + OH = ISOP1N23O4OH + OH : 8.38e-12*exp(390/T)*0.76*[1/(2.28e-20*[M]+1)];\n
 ISOP1N2OOH + OH = ISOP1N2OOH3OO4OH : 8.38e-12*exp(390/T)*0.276;\n
 SOP1N4OOH + OH = ISOP1N2OH34O + OH : 2.24e-11*exp(390/T)*0.31*[1/(2.185e-20*[M]+1)];\n
 ISOP1N4OOH + OH = ISOP1N2OH3OO4OOH : 2.24e-11*exp(390/T)*0.109;\n
 IISOP1N4OOH + OH = ISOP1N2OO3OH4OOH : 2.24e-11*exp(390/T)*0.6;\n
 ISOP1N4OOH + OH = ISOP12O3OH4OOH + NO2 : 2.24e-11*exp(390/T)*0.69*[1/(2.715e-19*[M]+1)];\n
 ISOP3OOH4N + OH = ISOP1OH23O4N + OH : 1.17e-11*exp(390/T)*0.965*[1/(2.28e-20*[M]+1)];\n
 ISOP3OOH4N + OH = ISOP1OH2OO3OOH4N : 1.17e-11*exp(390/T)*0.35;\n
 ISOP1OOH4N + OH = ISOP12O3OH4N + OH : 3.07e-11*exp(390/T)*0.69*[1/(2.185e-20*[M]+1)];\n
 ISOP1OOH4N + OH = ISOP1OOH2OO3OH4N : 3.07e-11*exp(390/T)*0.243;\n
 ISOP1OOH4N + OH = ISOP1OOH2OH3OO4N : 3.07e-11*exp(390/T)*0.27;\n
 ISOP1OH23O4N + OH = ISOP1OOH2OH34O + NO2 : 3.07e-11*exp(390/T)*0.31*[1/(2.715e-19*[M]+1)];\n
 ISOP1N23O4OH + OH = ISOP1N23O4CO + HO2 : 4.78e-11*exp(-400/T)*0.24*0.2;\n
 ISOP1N23O4OH + OH = CH2O + NO2 + MVKENOL : 4.78e-11*exp(-400/T)*0.24*0.5*[1/(1.014e-20*[M]+1)];\n
 ISOP1N23O4OH + OH = ISOP1N2OH3OO4CO : 4.78e-11*exp(-400/T)*0.24*0.5*[1/(1.014e-20*[M]+1)];\n
 ISOP1OH23O4N + OH = ISOP1CO23O4N + HO2 : 4.78e-11*exp(-400/T)*0.24*0.2;\n
 ISOP1OH23O4N + OH = CH2O + NO2 + MCRENOL : 4.78e-11*exp(-400/T)*0.24*0.5*[1/(1.014e-20*[M]+1)];\n
 ISOP1OH23O4N + OH = ISOP1CO2OO3OH4N : 4.78e-11*exp(-400/T)*0.24*0.5*[1/(1.014e-20*[M]+1)];\n
 ISOP12O3OH4N + OH = ISOP12O3CO4N + HO2 : 0.8*0.2*3.22e-11*exp(-400/T);\n
 ISOP12O3OH4N + OH = ISOP1OH3OH4CO + NO2 : 0.8*0.4*3.22e-11*exp(-400/T);\n
 ISOP12O3OH4N + OH = ISOP1OH2OO3CO4N : 0.8*3.22e-11*exp(-400/T)*[1/(6.09e-20*[M]+1)];\n

ISOP1N4CO + OH = NO2 + ISOP12O344CO : $4.13e-12 \cdot \exp(470/T) \cdot [1/(1.623e-19 \cdot [M]+1)]$;\

ISOP1N4CO + OH = ISOP1N2OO344CO : $0.7 \cdot 4.13e-12 \cdot \exp(470/T)$;\

ISOP1N4CO + OH = ISOP1N4CO4OO : $0.1 \cdot 4.13e-12 \cdot \exp(470/T)$;\

ISOP1CO4N + OH = NO2 + ISOP121CO34O : $4.13e-12 \cdot \exp(470/T) \cdot [1/(1.623e-19 \cdot [M]+1)]$;\

ISOP1CO4N + OH = ISOP121CO3OO4N : $0.7 \cdot 4.13e-12 \cdot \exp(470/T)$;\

ISOP1CO4N + OH = ISOP1CO1OO4N : $0.1 \cdot 4.13e-12 \cdot \exp(470/T)$;\

ISOP1N4CO + OH = ISOP1N2OO3OH4CO : $2.24e-11 \cdot \exp(390/T) \cdot 0.6$;\

ISOP1N4CO + OH = ISOP12O3OH4CO + NO2 : $2.24e-11 \cdot \exp(390/T) \cdot 0.69 \cdot [1/(2.715e-19 \cdot [M]+1)]$;\

ISOP1CO4N + OH = ISOP1CO2OH34O + NO2 : $3.07e-11 \cdot \exp(390/T) \cdot 0.31 \cdot [1/(2.715e-19 \cdot [M]+1)]$;\

ISOP1CO4N + OH = ISOP1CO2OH3OO4N : $3.07e-11 \cdot \exp(390/T) \cdot 0.27$;\

ISOP1N4OHc + OH = ISOP12O3OH4OH : $2.24e-11 \cdot \exp(390/T) \cdot 0.69 \cdot [1/(2.715e-19 \cdot [M]+1)]$;\

ISOP1N4OHc + OH = ISOP1N2OO3OH4OH : $2.24e-11 \cdot \exp(390/T) \cdot 0.69 \cdot 0.87$;\

ISOP1N4OHt + OH = ISOP12O3OH4OH : $2.24e-11 \cdot \exp(390/T) \cdot 0.69 \cdot [1/(2.715e-19 \cdot [M]+1)]$;\

ISOP1N4OHt + OH = ISOP1N2OO3OH4OH : $2.24e-11 \cdot \exp(390/T) \cdot 0.69 \cdot 0.87$;\

ISOP1OH4Nc + OH = ISOP1OH2OH34O : $3.07e-11 \cdot \exp(390/T) \cdot 0.31 \cdot [1/(2.715e-19 \cdot [M]+1)]$;\

ISOP1OH4Nc + OH = ISOP1OH2OH3OO4N : $3.07e-11 \cdot \exp(390/T) \cdot 0.31 \cdot 0.87$;\

ISOP1OH4Nt + OH = ISOP1OH2OH34O : $3.07e-11 \cdot \exp(390/T) \cdot 0.31 \cdot [1/(2.715e-19 \cdot [M]+1)]$;\

ISOP1OH4Nt + OH = ISOP1OH2OH3OO4N : $3.07e-11 \cdot \exp(390/T) \cdot 0.31 \cdot 0.87$;\