

Table S1. List of new model species from the SAPRC-11 mechanism.

Type and Name	Description
Active Radical Species and Operators	
MEO2	Methyl Peroxy Radicals
RO2C	Peroxy Radical Operator representing NO to NO2 and NO3 to NO2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals.
RO2XC	Peroxy Radical Operator representing NO consumption (used in conjunction with organic nitrate formation), and the effects of peroxy radical reactions on NO3, acyl peroxy radicals, and other peroxy radicals.
MECO3	Acetyl Peroxy Radicals
RCO3	Peroxy Propionyl and higher peroxy acyl Radicals
BZCO3	Peroxyacetyl radical formed from Aromatic Aldehydes
MACO3	Peroxyacetyl radicals formed from methacrolein and other acroleins.
Steady State Radical Species	
BZO	Phenoxy Radicals
HCOCO3	HC(O)C(O)OO Radicals
PBZN	PAN analogues formed from Aromatic Aldehydes
Explicit and Lumped Molecule Reactive Organic Product Species	
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes (mechanism based on propionaldehyde)
ACET	Acetone
MEOH	Methanol
HCOOH	Formic Acid
CCOOH	Acetic Acid. Also used for peroxyacetic acid.
RCOOH	Higher organic acids and peroxy acids (mechanism based on propionic acid)
COOH	Methyl Hydroperoxide
ROOH	Lumped organic hydroperoxides with 2-4 carbons. Mechanism based on that estimated for npropyl hydroperoxide.
R6OOH	Lumped organic hydroperoxides with 5 or more carbons, and organic hydroperoxides formed from aromatics that do not participate in SOA formation. Mechanism based on that estimated for 3-hexyl hydroperoxide.
RAOOH	Organic hydroperoxides formed from aromatic hydrocarbons that condense to form SOA (see Carter et al, 2012 for a complete listing of the mechanism and model species used for modeling aromatic SOA formation.)
GLY	Glyoxal
BACL	Biacetyl
PHEN	Phenol
CRES	Cresols
XYNL	Xylenols and higher alkylphenols
CATL	Catechols
NPHE	Nitrophenols
BALD	Aromatic aldehydes (e.g., benzaldehyde)

MACR	Methacrolein
MVK	Methyl Vinyl Ketone
IPRD	Lumped isoprene product species
Aromatic unsaturated ring fragmentation products	
AFG1	Monounsaturated dialdehydes or aldehyde-ketones formed from aromatics. - Most photoreactive
AFG2	Monounsaturated dialdehydes or aldehyde-ketones formed from aromatics. - Least photoreactive
AFG3	Diunsaturated dicarbonyl aromatic fragmentation products that are assumed not to photolyze rapidly
Lumped Parameter Products	
PROD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than $5 \times 10^{-12} \text{ cm}^3 \text{ molec}^{-2} \text{ sec}^{-1}$.
RNO3	Lumped Organic Nitrates
Steady state operators used to represent radical or product formation in peroxy radical reactions.	
xHO2	Formation of HO2 from alkoxy radicals formed in peroxy radical reactions with NO and NO3 (100% yields) and RO2 (50% yields)
xOH	As above, but for OH
xNO2	As above, but for NO2
xMEO2	As above, but for MEO2
xMECO3	As above, but for MECO3
xRCO3	As above, but for RCO3
xMACO3	As above, but for MACO3
xCO	As above, but for CO
xHCHO	As above, but for HCHO
xCCHO	As above, but for CCHO
xRCHO	As above, but for RCHO
xACET	As above, but for ACET
xMEK	As above, but for MEK
xPROD2	As above, but for PROD2
xBALD	As above, but for BALD
xGLY	As above, but for GLY
xMGLY	As above, but for MGLY
xBACL	As above, but for BACL
xAFG1	As above, but for AFG1
xAFG2	As above, but for AFG2
xAFG4	As above, but for AFG4
xMACR	As above, but for MACR
xMVK	As above, but for MVK
xIPRD	As above, but for IPRD
xRNO3	As above, but for RNO3
zRNO3	Formation of RNO3 in the RO2 + NO, reaction, or formation of corresponding non-nitrate products (represented by PROD2) formed from alkoxy radicals formed in RO2 + NO3 and (in 50% yields) RO2 + RO2 reactions.
yROOH	Formation of ROOH following RO2 + HO2 reactions, or formation of H-shift disproportionation products (represented by MEK) in the RO2 + RCO3 and (in 50% yields) RO2 + RO2 reactions.

yR6OOH	As above, but the RO ₂ + HO ₂ product is represented by R6OOH and the H-shift products are represented by PROD2.
yRAOOH	Like yROOH or yR6OOH but for RAOOH
Non-Reacting Species	
XC	Lost Carbon or carbon in unreactive products
XN	Lost Nitrogen or nitrogen in unreactive products

Table S2. Listing of new reactions and rate parameters from the base SAPRC-11 mechanism.

Label	Label Reaction and Products	Rate Parameters			
		k(300)	A	Ea	B
Methyl peroxy and methoxy reactions					
BR01	MEO2 + NO = NO2 + HCHO + HO2	7.64e-12	2.30e-12	-0.72	
BR02	MEO2 + HO2 = COOH + O2	4.65e-12	3.46e-13	-1.55	0.36
BR03	MEO2 + HO2 = HCHO + O2 + H2O	4.50e-13	3.34e-14	-1.55	-3.53
BR04	MEO2 + NO3 = HCHO + HO2 + NO2	1.30e-12			
BR05	MEO2 + MEO2 = ME OH + HCHO + O2	2.16e-13	6.39e-14	-0.73	-1.80
BR06	MEO2 + MEO2 = #2 {HCHO + HO2}	1.31e-13	7.40e-13	1.03	
Active Peroxy Radical Operators					
BR07	RO2C + NO = NO2	9.23e-12	2.60e-12	-0.76	
BR08	RO2C + NO3 = NO2	2.30e-12			
BR09	RO2C + MEO2 = #.5 HO2 + #.75 HCHO + #.25 ME OH	2.00e-13			
BR10	RO2XC + NO = XN	Same k as rxn BR07			
BR11	RO2XC + NO3 = NO2	Same k as rxn BR08			
BR12	RO2XC + MEO2 = #.5 HO2 + #.75 HCHO + #.25 ME OH	Same k as rxn BR09			
Reactions of Acyl Peroxy Radicals, PAN, and PAN analogues					
BR13	MECO3 + NO2 = PAN	9.37e-12			
BR14	MECO3 + NO = MEO2 + CO2 + NO2	1.97e-11	7.50e-12	-0.58	
BR15	MECO3 + HO2 = #.44 {OH + MEO2 + CO2} + #.41 CCOOH + #.15 {O3 + CCOOH}	1.36e-11	5.20e-13	-1.95	
BR16	MECO3 + NO3 = MEO2 + CO2 + NO2 + O2	Same k as rxn BR08			
BR17	MECO3 + MEO2 = #.1 {CCOOH + HCHO + O2} + #.9 {HCHO + HO2 + MEO2 + CO2}	1.06e-11	2.00e-12	-0.99	
BR18	MECO3 + RO2C = MEO2 + CO2	1.56e-11	4.40e-13	-2.13	
BR19	MECO3 + RO2XC = MEO2 + CO2	Same k as rxn BR18			
BR20	MECO3 + MECO3 = #2 {MEO2 + CO2} + O2	1.54e-11	2.90e-12	-0.99	
BR21	RCO3 + NO = NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2	2.08e-11	6.70e-12	-0.68	
BR22	RCO3 + HO2 = #.44 {OH + RO2C + xHO2 + xCCHO + yROOH + CO2} + #.41 RCOOH + #.15 {O3 + RCOOH}	Same k as rxn BR15			
BR23	RCO3 + NO3 = NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2 + O2	Same k as rxn BR08			
BR24	RCO3 + MEO2 = HCHO + HO2 + RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR17			
BR25	RCO3 + RO2C = RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR18			
BR26	RCO3 + RO2XC = RO2C + xHO2 + xCCHO + yROOH + CO2	Same k as rxn BR18			
BR27	RCO3 + MECO3 = #2 CO2 + MEO2 + RO2C + xHO2 + yROOH + xCCHO + O2	Same k as rxn BR20			
BR28	RCO3 + RCO3 = #2 {RO2C + xHO2 + xCCHO + yROOH + CO2}	Same k as rxn BR20			
BR29	BZCO3 + NO2 = PBZN	1.37e-11			
BR30	PBZN = BZCO3 + NO2	4.27e-4	7.90e+16	27.82	
BR31	PBZN + HV = #.6 {BZCO3 + NO2} + #.4 {CO2 + BZO + RO2C + NO3}	Phot Set= PAN			
BR32	BZCO3 + NO = NO2 + CO2 + BZO + RO2C	Same k as rxn BR21			
BR33	BZCO3 + HO2 = #.44 {OH + BZO + RO2C +	Same k as rxn BR15			

	$\text{CO}_2\} + \# .41 \text{RCOOH} + \# .15 \{\text{O}_3 + \text{RCOOH},$ + #2.24 XC				
BR34	$\text{BZCO}_3 + \text{NO}_3 = \text{NO}_2 + \text{CO}_2 + \text{BZO} + \text{RO}_2\text{C} + \text{O}_2$	Same k as rxn BR08			
BR35	$\text{BZCO}_3 + \text{MEO}_2 = \text{HCHO} + \text{HO}_2 + \text{RO}_2\text{C} + \text{BZO} + \text{CO}_2$	Same k as rxn BR17			
BR36	$\text{BZCO}_3 + \text{RO}_2\text{C} = \text{RO}_2\text{C} + \text{BZO} + \text{CO}_2$	Same k as rxn BR18			
BR37	$\text{BZCO}_3 + \text{RO}_2\text{XC} = \text{RO}_2\text{C} + \text{BZO} + \text{CO}_2$	Same k as rxn BR18			
BR38	$\text{BZCO}_3 + \text{MECO}_3 = \# 2 \text{CO}_2 + \text{MEO}_2 + \text{BZO} + \text{RO}_2\text{C}$	Same k as rxn BR20			
BR39	$\text{BZCO}_3 + \text{RCO}_3 = \# 2 \text{CO}_2 + \text{RO}_2\text{C} + x\text{HO}_2 + y\text{ROOH} + x\text{CCHO} + \text{BZO} + \text{RO}_2\text{C}$	Same k as rxn BR20			
BR40	$\text{BZCO}_3 + \text{BZCO}_3 = \# 2 \{\text{BZO} + \text{RO}_2\text{C} + \text{CO}_2\}$	Same k as rxn BR20			
BR42	$\text{MACO}_3 + \text{NO} = \text{NO}_2 + \text{CO}_2 + \text{HCHO} + \text{MECO}_3$	Same k as rxn BR21			
BR43	$\text{MACO}_3 + \text{HO}_2 = \# .44 \{\text{OH} + \text{HCHO} + \text{MECO}_3 + \text{CO}_2\} + \# .41 \text{RCOOH} + \# .15 \{\text{O}_3 + \text{RCOOH}\} + \# .56 \text{XC}$	Same k as rxn BR15			
BR44	$\text{MACO}_3 + \text{NO}_3 = \text{NO}_2 + \text{CO}_2 + \text{HCHO} + \text{MECO}_3 + \text{O}_2$	Same k as rxn BR08			
BR45	$\text{MACO}_3 + \text{MEO}_2 = \# 2 \text{HCHO} + \text{HO}_2 + \text{CO}_2 + \text{MECO}_3$	Same k as rxn BR17			
BR46	$\text{MACO}_3 + \text{RO}_2\text{C} = \text{CO}_2 + \text{HCHO} + \text{MECO}_3$	Same k as rxn BR18			
BR47	$\text{MACO}_3 + \text{RO}_2\text{XC} = \text{CO}_2 + \text{HCHO} + \text{MECO}_3$	Same k as rxn BR18			
BR48	$\text{MACO}_3 + \text{MECO}_3 = \# 2 \text{CO}_2 + \text{MEO}_2 + \text{HCHO} + \text{MECO}_3 + \text{O}_2$	Same k as rxn BR20			
BR49	$\text{MACO}_3 + \text{RCO}_3 = \text{HCHO} + \text{MECO}_3 + \text{RO}_2\text{C} + x\text{HO}_2 + y\text{ROOH} + x\text{CCHO} + \# 2 \text{CO}_2$	Same k as rxn BR20			
BR50	$\text{MACO}_3 + \text{BZCO}_3 = \text{HCHO} + \text{MECO}_3 + \text{BZO} + \text{RO}_2\text{C} + \# 2 \text{CO}_2$	Same k as rxn BR20			
BR51	$\text{MACO}_3 + \text{MACO}_3 = \# 2 \{\text{HCHO} + \text{MECO}_3 + \text{CO}_2\}$	Same k as rxn BR20			
Other Organic Radical Species					
BR52	$\text{BZO} + \text{NO}_2 = \text{NPHE}$	3.79e-11	2.30e-11	-0.30	
BR53	$\text{BZO} + \text{HO}_2 = \text{CRES} + \# -1 \text{XC}$	7.63e-12	3.80e-13	-1.79	
BR54	$\text{BZO} = \text{CRES} + \text{RO}_2\text{C} + x\text{HO}_2 + \# -1 \text{XC}$	1.00e-3			
Explicit and Lumped Molecule Organic Products					
BP01	$\text{CCHO} + \text{OH} = \text{MECO}_3 + \text{H}_2\text{O}$	1.49e-11	4.40e-12	-0.73	
BP02	$\text{CCHO} + \text{HV} = \text{CO} + \text{HO}_2 + \text{MEO}_2$	Phot Set= CCHO_R			
BP03	$\text{CCHO} + \text{NO}_3 = \text{HNO}_3 + \text{MECO}_3$	2.84e-15	1.40e-12	3.70	
BP04	$\text{RCHO} + \text{OH} = \# .965 \text{RCO}_3 + \# .035 \{\text{RO}_2\text{C} + x\text{HO}_2 + x\text{CO} + x\text{CCHO} + y\text{ROOH}\}$	1.97e-11	5.10e-12	-0.80	
BP05	$\text{RCHO} + \text{HV} = \text{RO}_2\text{C} + x\text{HO}_2 + y\text{ROOH} + x\text{CCHO} + \text{CO} + \text{HO}_2$	Phot Set= C2CHO			
BP06	$\text{RCHO} + \text{NO}_3 = \text{HNO}_3 + \text{RCO}_3$	6.74e-15	1.40e-12	3.18	
BP07	$\text{ACET} + \text{OH} = \text{RO}_2\text{C} + x\text{MECO}_3 + x\text{HCHO} + y\text{ROOH}$	1.91e-13	4.56e-14	-0.85	3.65
BP08	$\text{ACET} + \text{HV} = \# .62 \text{MECO}_3 + \# 1.38 \text{MEO}_2 + \# .38 \text{CO}$	Phot Set= ACET-06, qy= 0.5			
BP09	$\text{MEOH} + \text{OH} = \text{HCHO} + \text{HO}_2$	9.02e-13	2.85e-12	0.69	
BP10	$\text{CCOOH} + \text{OH} = \# .509 \text{MEO}_2 + \# .491 \text{RO}_2\text{C} + \# .509 \text{CO}_2 + \# .491 x\text{HO}_2 + \# .491 x\text{MGLY} + \# .491 y\text{ROOH} + \# -.491 \text{XC}$	7.26e-13	4.20e-14	-1.70	
BP11	$\text{COOH} + \text{OH} = \text{H}_2\text{O} + \# .3 \{\text{HCHO} + \text{OH}\} +$	7.40e-12	3.80e-12	-0.40	

	#.7 MEO2				
BP12	COOH + HV = HCHO + HO2 + OH	Phot Set= COOH			
BP13	MACR + OH = #.5 MACO3 + #.5 {RO2C + xHO2} + #.416 xCO + #.084 xHCHO + #.416 xMEK + #.084 xMGLY + #.5 yROOH + #-.416 XC	2.84e-11	8.00e-12	-0.76	
BP14	MACR + O3 = #.208 OH + #.108 HO2 + #.1 RO2C + #.45 CO + #.117 CO2 + #.1 HCHO + #.9 MGLY + #.333 HCOOH + #.1 xRCO3 + #.1 xHCHO + #.1 yROOH + #-0.1 XC	1.28e-18	1.40e-15	4.17	
BP15	MACR + NO3 = #.5 {MACO3 + RO2C + HNO3 + xHO2 + xCO} + #.5 yROOH + #1.5 XC + #.5 XN	3.54e-15	1.50e-12	3.61	
BP16	MACR + HV = #.33 OH + #.67 HO2 + #.34 MECO3 + #.33 MACO3 + #.33 RO2C + #.67 CO + #.34 HCHO + #.33 xMECO3 + #.33 xHCHO + #.33 yROOH	Phot Set= MACR-06			
BP17	MVK + OH = #.975 RO2C + #.025 {RO2XC + zRNO3} + #.3 xHO2 + #.675 xMECO3 + #.3 xHCHO + #.675 xRCHO + #.3 xMGLY + yROOH + #-0.725 XC	1.99e-11	2.60e-12	-1.21	
BP18	MVK + O3 = #.164 OH + #.064 HO2 + #.05 {RO2C + xHO2} + #.475 CO + #.124 CO2 + #.05 HCHO + #.95 MGLY + #.351 HCOOH + #.05 xRCO3 + #.05 xHCHO + #.05 yROOH + #-0.05 XC	5.36e-18	8.50e-16	3.02	
BP19	MVK + NO3 = #4 XC + XN	Slow			
BP20	MVK + HV = #.4 MEO2 + #.6 CO + #.6 PROD2 + #.4 MACO3 + #-2.2 XC	Phot Set= MVK-06			
BP21	IPRD + OH = #.289 MACO3 + #.67 {RO2C + xHO2} + #.041 {RO2XC + zRNO3} + #.336 xCO + #.055 xHCHO + #.129 xCCHO + #.013 xRCHO + #.15 xMEK + #.332 xPROD2 + #.15 xGLY + #.174 xMGLY + #-0.504 XC + #.711 yR6OOH	6.19e-11			
BP22	IPRD + O3 = #.285 OH + #.4 HO2 + #.048 {RO2C + xRCO3} + #.498 CO + #.14 CO2 + #.124 HCHO + #.21 MEK + #.023 GLY + #.742 MGLY + #.1 HCOOH + #.372 RCOOH + #.047 xCCHO + #.001 xHCHO + #.048 yR6OOH + #.329 XC	4.18e-18			
BP23	IPRD + NO3 = #.15 {MACO3 + HNO3} + #.799 {RO2C + xHO2} + #.051 {RO2XC + zRNO3} + #.572 xCO + #.227 xHCHO + #.218 xRCHO + #.008 xMGLY + #.572 xRNO3 + #.85 yR6OOH + #.278 XN + #-.815 XC	1.00e-13			
BP24	IPRD + HV = #1.233 HO2 + #.467 MECO3 + #.3 RCO3 + #1.233 CO + #.3 HCHO + #.467 CCHO + #.233 MEK + #-.233 XC	Phot Set= MACR-06			
Lumped Parameter Organic Products					
BP25	PROD2 + OH = #.472 HO2 + #.379 xHO2 + #.029 xMECO3 + #.049 xRCO3 + #.473 RO2C + #.071 RO2XC + #.071 zRNO3 + #.002 HCHO + #.211 xHCHO + #.001 CCHO + #.083 xCCHO + #.143 RCHO + #.402 xRCHO + #.115 xMEK + #.329 PROD2 + #.007 xPROD2 + #.528 yR6OOH + #.877 XC	1.55e-11			

BP26	PROD2 + HV = #.913 xHO2 + #.4 MECO3 + #.6 RCO3 + #1.59 RO2C + #.087 RO2XC + #.087 zRNO3 + #.303 xHCHO + #.163 xCCHO + #.78 xRCHO + yR6OOH + #- .091 XC	Phot Set= MEK-06, qy= 4.86e-3			
Aromatic Products					
BP27	GLY + HV = #2 {CO + HO2}	Phot Set= GLY-07R			
BP28	GLY + HV = HCHO + CO	Phot Set= GLY-07M			
BP29	GLY + OH = #.7 HO2 + #1.4 CO + #.3 HCOCO3	9.63e-12	3.10e-12	-0.68	
BP30	GLY + NO3 = HNO3 + #.7 HO2 + #1.4 CO + #.3 HCOCO3	1.02e-15	2.80e-12	4.72	
BP31	HCOCO3 + NO = HO2 + CO + CO2 + NO2	Same k as rxn BR21			
BP32	HCOCO3 + NO2 = HO2 + CO + CO2 + NO3	1.21e-11	1.21e-11	0.0	-1.07
BP33	HCOCO3 + HO2 = #.44 {OH + HO2 + CO + CO2} + #.56 GLY + #.15 O3	Same k as rxn BR15			
BP34	BACL + HV = #2 MECO3	Phot Set= BACL-07			
BP35	NPHE + OH = BZO + XN	3.50e-12			
BP36	NPHE + HV = HONO + #6 XC	Phot Set= NO2-06, qy= 1.5e-3			
BP37	NPHE + HV = #6 XC + XN	Phot Set= NO2-06, qy= 1.5e-2			
BP38	BALD + OH = BZCO3	1.20e-11			
BP39	BALD + HV = #7 XC	Phot Set= BALD-06, qy= 0.06			
BP40	BALD + NO3 = HNO3 + BZCO3	2.73e-15	1.34e-12	3.70	
BP41	PHEN + OH = #.7 HO2 + #.1 BZO + #.095 xHO2 + #.105 OH + #.095 RO2C + #.7 CATL + #.105 AFG3 + #.048 xAFG1 + #.048 xAFG2 + #.095 xGLY + #.095 yRAOOH	2.74e-11	4.70e-13	-2.42	
BP42	PHEN + NO3 = #.1 HNO3 + #.9 XN + #.7 HO2 + #.1 BZO + #.095 xHO2 + #.105 OH + #.095 RO2C + #.7 CATL + #.105 AFG3 + #.048 xAFG1 + #.048 xAFG2 + #.095 xGLY + #.095 yRAOOH	3.80e-12			
BP43	CRES + OH = #.7 HO2 + #.1 BZO + #.17 xHO2 + #.03 OH + #.17 RO2C + #.7 CATL + #.03 AFG3 + #.085 xAFG1 + #.085 xAFG2 + #.085 xGLY + #.085 xMGLY + #.17 yRAOOH	4.06e-11	1.60e-12	-1.93	
BP44	CRES + NO3 = #.1 HNO3 + #.9 XN + #.7 HO2 + #.1 BZO + #.17 xHO2 + #.03 OH + #.17 RO2C + #.7 CATL + #.03 AFG3 + #.085 xAFG1 + #.085 xAFG2 + #.085 xGLY + #.085 xMGLY + #.170 yRAOOH	1.40e-11			
BP45	XYNL + OH = #.7 HO2 + #.07 BZO + #.23 xHO2 + #.23 RO2C + #.7 CATL + #.115 xAFG1 + #.115 xAFG2 + #.115 xGLY + #.115 xMGLY + #.23 yRAOOH	7.38e-11			
BP46	XYNL + NO3 = #.07 HNO3 + #.93 XN + #.7 HO2 + #.07 BZO + #.23 xHO2 + #.23 RO2C + #.7 CATL + #.115 xAFG1 + #.115 xAFG2 + #.115 xGLY + #.115 xMGLY + #.23 yRAOOH	3.06e-11			
BP47	CATL + OH = #.4 HO2 + #.2 BZO + #.2 xHO2 + #.2 OH + #.2 RO2C + #.2 AFG3 + #.1 xAFG1 + #.1 xAFG2 + #.1 xGLY + #.1 xMGLY + #.33 CNDPP + #.2 yRAOOH	2.00e-10			

BP48	CATL + NO3 = #.2 HNO3 + #.8 XN + #.4 HO2 + #.2 BZO + #.2 xHO2 + #.2 OH + #.2 RO2C + #.2 AFG3 + #.1 xAFG1 + #.1 xAFG2 + #.1 xGLY + #.1 xMGLY + #.2 yRAOOH	1.70e-10			
BP49	AFG1 + OH = #.217 MACO3 + #.723 RO2C + #.060 {RO2XC + zRNO3} + #.521 xHO2 + #.201 xMECO3 + #.334 xCO + #.407 xRCHO + #.129 xMEK + #.107 xGLY + #.267 xMGLY + #.783 yR6OOH + #.284 XC	7.40e-11			
BP50	AFG1 + HV = #1.023 HO2 + #.173 MEO2 + #.305 MECO3 + #.500 MACO3 + #.695 CO + #.195 GLY + #.305 MGLY + #.217 XC	Phot Set= AFG1			
BP51	AFG2 + OH = #.217 MACO3 + #.723 RO2C + #.060 {RO2XC + zRNO3} + #.521 xHO2 + #.201 xMECO3 + #.334 xCO + #.407 xRCHO + #.129 xMEK + #.107 xGLY + #.267 xMGLY + #.783 yR6OOH + #.284 XC	7.40e-11			
BP52	AFG2 + HV = PROD2 + #-1 XC	Phot Set= AFG1			
BP53	AFG3 + OH = #.206 MACO3 + #.733 RO2C + #.117 {RO2XC + zRNO3} + #.561 xHO2 + #.117 xMECO3 + #.114 xCO + #.274 xGLY + #.153 xMGLY + #.019 xBACL + #.195 xAFG1 + #.195 xAFG2 + #.231 xIPRD + #.794 yR6OOH + #.938 XC	9.35e-11			
BP54	AFG3 + O3 = #.471 OH + #.554 HO2 + #.013 MECO3 + #.258 RO2C + #.007 {RO2XC + zRNO3} + #.580 CO + #.190 CO2 + #.366 GLY + #.184 MGLY + #.350 AFG1 + #.350 AFG2 + #.139 AFG3 + #.003 MACR + #.004 MVK + #.003 IPRD + #.095 xHO2 + #.163 xRCO3 + #.163 xHCHO + #.095 xMGLY + #.264 yR6OOH + #-.575 XC	1.43e-17			
BP55	RAOOH + OH = #.139 OH + #.148 HO2 + #.589 RO2C + #.124 RO2XC + #.124 zRNO3 + #.074 PROD2 + #.147 MGLY + #.139 IPRD + #.565 xHO2 + #.024 xOH + #.448 xRCHO + #.026 xGLY + #.030 xMEK + #.252 xMGLY + #.073 xAFG1 + #.073 xAFG2 + #.713 yR6OOH + #1.674 XC	1.41e-10			
BP56	RAOOH + HV = OH + HO2 + #.5 {GLY + MGLY + AFG1 + AFG2} + #-.5 XC	Phot Set= COOH			
Aromatic VOCs represented in chamber simulations					
BE01	BENZENE + OH = #.027 RO2XC + #.31 RO2C + #.57 HO2 + #.31 xHO2 + #.027 zRNO3 + #.57 PHEN + #.31 xGLY + #.183 xAFG1 + #.127 xAFG2 + #.337 yRAOOH + #.093 OH + #.093 AFG3 + #-.403 XC	1.22e-12	2.33e-12	0.38	
BE02	TOLUENE + OH = #.074 RO2XC + #.605 RO2C + #.18 HO2 + #.605 xHO2 + #.074 zRNO3 + #.073 yR6OOH + #.065 xBALD + #.18 CRES + #.29 xGLY + #.25 xMGLY + #.324 xAFG1 + #.216 xAFG2 + #.606 yRAOOH + #.141 OH + #.141 AFG3 + #-.176 XC	5.58e-12	1.81e-12	-0.67	
BE03	XYLENE + OH = #.098 RO2XC + #.6 RO2C + #.11 HO2 + #.6 xHO2 + #.098 zRNO3 + #.046 yR6OOH + #.04 xBALD + #.11 XYNL + #.11 xGLY + #.45 xMGLY + #.319 xAFG1 + #.241 xAFG2 + #.651 yRAOOH + #.192	2.31e-11			

	OH + #.192 AFG3 + #.538 XC				
Steady-State Peroxy Radical operators (for formation of inorganic and radical products)					
RO01	xHO2 = HO2	k is variable parameter: RO2RO ¹			
RO02	xHO2 =	k is variable parameter: RO2XRO ²			
RO03	xOH = OH	k is variable parameter: RO2RO			
RO04	xOH =	k is variable parameter: RO2XRO			
RO05	xNO2 = NO2	k is variable parameter: RO2RO			
RO06	xNO2 = XN	k is variable parameter: RO2XRO			
RO07	xMEO2 = MEO2	k is variable parameter: RO2RO			
RO08	xMEO2 = XC	k is variable parameter: RO2XRO			
RO09	xMECO3 = MECO3	k is variable parameter: RO2RO			
RO10	xMECO3 = #2 XC	k is variable parameter: RO2XRO			
RO11	xRCO3 = RCO3	k is variable parameter: RO2RO			
RO12	xRCO3 = #3 XC	k is variable parameter: RO2XRO			
RO13	xMACO3 = MACO3	k is variable parameter: RO2RO			
RO14	xMACO3 = #4 XC	k is variable parameter: RO2XRO			
RO15	xCO = CO	k is variable parameter: RO2RO			
RO16	xCO = XC	k is variable parameter: RO2XRO			
Steady-State Peroxy Radical operators (for formation of organic product species)					
PO01	xHCHO = HCHO	k is variable parameter: RO2RO			
PO02	xHCHO = XC	k is variable parameter: RO2XRO			
PO03	xCCHO = CCHO	k is variable parameter: RO2RO			
PO04	xCCHO = #2 XC	k is variable parameter: RO2XRO			
PO05	xRCHO = RCHO	k is variable parameter: RO2RO			
PO06	xRCHO = #3 XC	k is variable parameter: RO2XRO			
PO07	xACET = ACET	k is variable parameter: RO2RO			
PO08	xACET = #3 XC	k is variable parameter: RO2XRO			
PO09	xMEK = MEK	k is variable parameter: RO2RO			
PO10	xMEK = #4 XC	k is variable parameter: RO2XRO			
PO11	xPROD2 = PROD2	k is variable parameter: RO2RO			
PO12	xPROD2 = #6 XC	k is variable parameter: RO2XRO			
PO13	xMACR = MACR	k is variable parameter: RO2RO			
PO14	xMACR = #4 XC	k is variable parameter: RO2XRO			
PO15	xMVK = MVK	k is variable parameter: RO2RO			
PO16	xMVK = #4 XC	k is variable parameter: RO2XRO			
PO17	xIPRD = IPRD	k is variable parameter: RO2RO			
PO18	xIPRD = #5 XC	k is variable parameter: RO2XRO			
PO19	xRNO3 = RNO3	k is variable parameter: RO2RO			
PO20	xRNO3 = #6 XC + XN	k is variable parameter: RO2XRO			
PO21	xGLY = GLY	k is variable parameter: RO2RO			
PO22	xGLY = #2 XC	k is variable parameter: RO2XRO			
PO23	xMGLY = MGLY	k is variable parameter: RO2RO			
PO24	xMGLY = #3 XC	k is variable parameter: RO2XRO			
PO25	xBACL = BACL	k is variable parameter: RO2RO			
PO26	xBACL = #4 XC	k is variable parameter: RO2XRO			
PO27	xBALD = BALD	k is variable parameter: RO2RO			
PO28	xBALD = #7 XC	k is variable parameter: RO2XRO			
PO29	xAFG1 = AFG1	k is variable parameter: RO2RO			
PO30	xAFG1 = #5 XC	k is variable parameter: RO2XRO			
PO31	xAFG2 = AFG2	k is variable parameter: RO2RO			
PO32	xAFG2 = #5 XC	k is variable parameter: RO2XRO			
PO33	xAFG4 = #6 XC	k is variable parameter: RO2XRO			
PO34	xAFG4 = AFG4	k is variable parameter: RO2RO			
PO35	zRNO3 = RNO3 + #-1 XN	k is variable parameter: RO2NO ³			
PO36	zRNO3 = PROD2 + HO2	k is variable parameter: RO2NN ⁴			
PO37	zRNO3 = #6 XC	k is variable parameter: RO2XRO			
PO38	yROOH = ROOH + #-3 XC	k is variable parameter: RO2HO2 ⁵			
PO39	yROOH = MEK + #-4 XC	k is variable parameter: RO2RO2M ⁶			

PO40	yROOH =	k is variable parameter: RO2RO
PO41	yR6OOH = R6OOH + #-6 XC	k is variable parameter: RO2HO2
PO42	yR6OOH = PROD2 + #-6 XC	k is variable parameter: RO2RO2M
PO43	yR6OOH =	k is variable parameter: RO2RO
PO44	yRAOOH = RAOOH + #-7 XC	k is variable parameter: RO2HO2
PO45	yRAOOH = PROD2 + #-6 XC	k is variable parameter: RO2RO2M
PO46	yRAOOH =	k is variable parameter: RO2RO

1. $RO2RO = k(RO2+NO)[NO] + k(RO2+NO3)[NO3] + k(RO2+MECO3)\{[MECO3]+[RCO3]+[BZCO3]+[MACO3]\} + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2)\{[RO2C]+[RO2XC]\}$
2. $RO2XRO = k(RO2+HO2)[HO2] + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2)\{[RO2C]+[RO2XC]\}$
3. $RO2NO = k(RO2+NO)[NO]$
4. $RO22NN = k(RO2+NO3)[NO3] + k(RO2+MECO3)\{[MECO3]+[RCO3]+[BZCO3]+[MACO3]\} + 0.5 k(RO2+MEO2)[MEO2] + 0.5 k(RO2+RO2)\{[RO2C]+[RO2XC]\}$
5. $RO2HO2 = k(RO2+HO2)[HO2]$
6. $RO2RO2M = 0.5 k(RO2+RO2)\{[RO2C]+[RO2XC]\}$