ASSESSMENT OF SAPRC07 WITH UPDATED ISOPRENE OXIDATION CHEMISTRY AGAINST OUTDOOR CHAMBER EXPERIMENTS

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ABSTRACT

Yuzhi Chen: Assessment of SAPRC07 with Updated Isoprene Oxidation Chemistry Against Outdoor Chamber Experiments
(Under the direction of William Vizuete)

Isoprene, the most emitted non-methane hydrocarbon, is known to influence ozone (O_3) formation in urban areas rich with biogenic emissions. To keep up with the recent advance on isoprene oxidation chemistry including the identification of isoprene epoxydiols (IEPOX) as a precursor to secondary organic aerosol (SOA), Xie et al. (2013) updated the SAPRC (Statewide Air Pollution Research Center)-07 chemical mechanism. It is currently unknown how the Xie modification of SAPRC07T impacts the ability of the model to predict O_3. In this project we will evaluate the Xie mechanism with simulations of 24 isoprene experiments from the UNC gas-phase chamber. Our results suggest that the new mechanism increases NO_X (nitrogen oxides) inter-conversion and produces more O3 than SAPRC07 for all experiments. In lower NO_X experiments, the new mechanism worsens O3 performance towards the wrong direction, increasing bias from 8.9% to 15.8%. We found increased NO_X recycling from NO_Z (oxidized NO_2) accounts for that. These results underline the importance of further studies on characterizing the NO_X recycling rate from isoprene nitrates.

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LIST OF ABBREVIATIONS

AQM	Air Quality Model
CH4	Methane
CMAQ	Community Multi-scale Air Quality Model
CO	Carbon Monoxide
EPA	U.S. Environmental Protection Agency
ETHE	Ethene
ETHLN	Model Species In The Xie Modification Of SAPRC07T Representing Ethanol Nitrate
HCHO	Formaldehyde
HO_2	Hydroperoxy radical
HO_X	Radical Family Including OH And HO_2
HPALD	Hydroperoxy-Aldehydes
IEPOX	Isoprene Epoxydiols
ISOP	Isoprene
ISOPNB	Model Species In The Xie Modification Of SAPRC07T Representing B-Isoprene Nitrates
ISOPND	Model Species In The Xie Modification Of SAPRC07T Representing Δ-Isoprene Nitrates
ISOPO2	Model Species In The Xie Modification Of SAPRC07T Representing Isoprene Peroxy radicals From Isoprene + OH
MACR	Model Species In SAPRC07 Representing Acroleins And Methacrolein
MACRN	Model Species In The Xie Modification Of SAPRC07T Representing Methacrolein Nitrate
MAE	Methacrylic Acid Epoxide
MEO2	Model Species In SAPRC07 Representing Methyl Peroxy Radicals
MECO3	Model Species In SAPRC07 Representing Acetyl Peroxy Radicals
MVK	Model species in SAPRC07 representing methyl vinyl ketone
MVKN	Model species in the Xie modification of SAPRC07T representing methyl vinyl ketone nitrate
NAAQS	National Ambient Air Quality Standards
NISOPO2	Model species in the Xie modification of SAPRC07T representing nitroxy peroxy radical from isoprene + NO_3

NISOPOOH	Model species in the Xie modification of SAPRC07T representing C5-nitrooxyhydroperoxide
NIT1	Model species in the Xie modification of SAPRC07T representing C5-nitrooxycarbonyl
NO	Nitric Oxide
NO_2	Nitrogen dioxide
NO_3	Nitrate Radical
NO_X	Nitrogen oxides including NO and NO_2
O_3	Ozone
OH	Hydroxyl Radical
PAN	Peroxy Acyl Nitrates
PM	Particulate Matter or aerosol
$PM_{2.5}$	Particulate Matter with aerodynamic diameter less than 2.5 micrometers
PROPNN	Model Species in Xie modification of SAPRC07T representing propanone nitrate
RNO3	Model Species in SAPRC07 representing lumped organic nitrates
RNO3I	Model Species in Xie modification of SAPRC07T representing lumped organic nitrates from isoprene
RO2C	Peroxy Radical operator in SAPRC07 representing NO to NO_2 and NO_3 to NO_2 conversions, and the effects of peroxy radical reactions on acyl peroxy and other peroxy radicals
SAPRC07	Statewide Air Pollution Research Center 2007 chemical mechanism
SO_2	Sulfur Dioxide
SOA	Secondary organic aerosol
VOC	Volatile Organic compound

CHAPTER I: INTRODUCTION

Isoprene (2-methyl-1, 3-butadiene, C_5H_8) is the most abundant non-methane hydrocarbon emitted from vegetation [1] and has a significant impact on atmospheric chemistry. Isoprene is known to influence ground-level ozone (O_3) formation in urban areas rich with biogenic emissions [2],[3]. In recent years new discoveries have been made concerning isoprene oxidation chemistry leading to SOA or PM formation [4]–[12]. By combining organic synthesis, computational calculations, smog chamber studies, and field measurements researchers have recently characterized reactive epoxides that are produced from the photochemical oxidation of isoprene and are significant for SOA formation [8]-[11]. These gas-phase oxidation products include MAE and IEPOX. From recent work it is clear that anthropogenic pollutants, such as NO_X and SO_2, significantly enhance these isoprene-derived epoxides as a source of $PM_{2.5}$ [8]-[12]. This is of great public health and regulatory importance since isoprene is primarily emitted from terrestrial vegetation, and thus, is not controllable, whereas anthropogenic emissions (e.g., NO_X, SO_2, or pre-existing primary aerosol) are controllable.

The chemical mechanisms in current regulatory models, however, do not have the gas-phase chemistry needed to predict isoprene-based SOA precursors. Isoprene gas phase oxidation chemistry is currently represented in AQMs in a condensed form. It is designed to represent the chemical formation of O_3 while incorporating simplification and approximation for computational efficiency. To evaluate future control strategies, new gas and particle phase isoprene chemistry must be incorporated in air quality models (AQMs) to study the importance of isoprene emissions on both ground level O_3 and SOA formation.

Xie et al. (2013) has developed a more explicit isoprene chemical mechanism with additional OH and NO3 oxidation pathways that produce SOA precursors. The mechanism is based on SAPRC07T [13], which adds hazardous air pollutants and precursors to secondary aerosols to the original SARPC07[14], [15]. In the original SAPRC07 mechanism, the reaction of isoprene with OH gives a product mixture including methacrolein (MACR) and methyl vinyl ketone (MVK) as shown below in R 1:

*ISOP + OH ----> 0.986*RO2C + 0.093*RO2XC*
*+ 0.093*zRNO3 + 0.907*xHO2*
*+ 0.624*xHCHO+ 0.23*xMACR*
*+ 0.32*xMVK + 0.357*xIPRD*
*+ yR6OOH + 0.167*XC* (R 1)

In the Xie modification, bulk hydroxyl-peroxy isoprene radicals ($ISOPO_2$) is formed (R 2), which in turn produces MACR and MVK by reaction with other species, namely, NO, HO_2, MEO2, RO2C, MECO3 and ISOPO2 itself (Reactions in Appendix A).

ISOP + OH ----> ISOPO2 + ISOPRXN (R 2)

In the original SAPRC07 mechanism, reaction with NO_3 does not yield either MACR or MVK, but in the Xie modification the product $NISOPO_2$ is created (R 3).

ISOP + NO3 → NISOPO2 (R 3)

NISOPO2, like its non-nitrated analogue, reacts with NO_3, NO, MEO_2, RO_2C, and $MECO_3$ to give small yields of MACR and MVK (Reactions in Appendix A). Other reactions of isoprene, with O_3 and Cl radicals, are unchanged in the Xie modification. Isoprene-derived nitrates are treated explicitly. First generation isoprene nitrates include ISOPN (= ISOPND + ISOPNB), NIT1, and NISOPOOH. ISOPND and ISOPNB are produced in the Xie mechanism instead of RNO3 in the standard SAPRC07. ISOPN reacts an order of magnitude faster with OH and has almost 100% higher recycling of NO_2 than RNO3 does. NIT1—formed in NISOPO2 + $NO/NO_3/RO_2$ reactions—reacts with OH and NO_3 and forms respective peroxy radical species, which react with other radicals similarly as the initially formed peroxy radical species (ISOPO2/NISOPO2) to yield little NO_X and other products. Xie also assumes 70% NO_X recycling efficiency from NIT1 + O_3 oxidation. NISOPOOH is the product of NISOPO2 + HO_2 reaction. The OH oxidation of the above first-generation nitrates forms secondary isoprene nitrates including: short-lived MVKN, MACRN, ETHLN, RNO3I, and longer-lived PROPNN. These products can either react with OH or photolyze to give NO_2 back. In the Xie mechanism, isoprene oxidation chemistry under low NO_X conditions was updated. These updates includes IEPOX formation from ISOPO2 + HO_2 channel (R 4) and HPALD formation from ISOPO2 isomerization (R 5). HO_X is produced in subsequent reactions of products from both reactions.

ISOPOOH + OH ----> IEPOX + OH (R 4)

ISOPO2 ----> HO2 + HPALD (R 5)

Xie et al. integrated the updated SAPRC07T chemical mechanism into the CMAQ model version 4.7 and simulated from 1 July to 16 August 2004 across the entire continental US and a portion of Canada and Mexico [13]. These additions to the CMAQ model allow for explicit predictions of OH reformation from isoprene peroxy radicals, NO_2 recycling from isoprene nitrates and IEPOX-SOA tracers (and thus total SOA mass from isoprene oxidation). Current AQMs estimate that isoprene contributes 27% [16] ~ 48% [17] to the global burden of SOA [18], yet under predict summertime isoprene SOA especially in areas like southeastern U.S. [19]. Xie et al. found that, compared to the base case simulation with SAPRC07T [20], their updated mechanism improves the simulation of aircraft measurement for gas phase compounds including NO_x (bias from -7% to 1%), O_3 (increases 1-2 ppbtv with bias still within ± 5%), HCHO (bias from -12% to -9%) and isoprene (bias from 26% to 4%). Xie also reported biogenic SOA increased by 15% compared to the base case.

The CMAQ results reported by Xie et al demonstrated improved model performance for several species, but large uncertainties still lie in the new gas phase chemistry. These uncertainties include isoprene nitrates yield from isoprene + OH/NO pathway and NO_X recycling efficiency from first-generation nitrates. Further, it is difficult to evaluate a chemical mechanism in AQMs, where other processes like transport, deposition and emissions act synergistically. The compensating errors from those processes might result in good agreement between observations and predictions and thus veil the real problems within the mechanism. To resolve this problem, smog chamber experiments are traditionally used to test and refine a new mechanism, or evaluate an existing mechanism [21]. The smog chamber is a closed and controlled system allowing for chemistry to be the main process that influences concentration. Thus, the discrepancy or agreement between observations and predictions are directly correlated with the mechanism being used. Condensed gas phase mechanisms are finely tuned engineering approximations for atmospheric chemistry. Xie et al. have added new reactions and species to the base mechanism and consequently have altered the radical budgets and nitrogen cycling. The Xie mechanism has yet to be evaluated against smog chamber experiments before being widely used in AQMs. Thus, it is currently unknown how the Xie modification of SAPRC07T impacts the ability of the model to predict O3, isoprene decay, and its oxidation products.

In this paper we will evaluate the Xie mechanism with simulations of experiments from the UNC outdoor smog chamber. A rich archive of chamber experiment data [22] provides this study with reliable measurements from 24 experiments conducted with isoprene and NO_X. These experiments were carried out for isoprene to NO_X concentration ratios (ISOP:NO_X) ranging from 0.18 to 9.29 in ppm/ppm, with initial NO_X concentrations from 0.17 ppm and 0.83 ppm. The focus will be on changes in model predictions from the SAPRAC07 mechanism that may have been introduced by the Xie et al. updates and evaluating the mechanism's ability to predict ozone.

CHAPTER II: METHODS

2.1 Modeling

Two mechanisms compared in this study, standard SAPRC07 [14], [15] and Xie, were implemented in the Morpho Photochemical Reaction Simulation System [23]. The SAPRC07 source code was created based on Dr. Carter's report [14], [15]. The Xie mechanism was contained in the CMAQ files provided by Dr. Xie, and converted to the Morpho format [24]. The UNC Auxiliary Mechanism (version-aadg) was used to account for chamber dependent wall effects. The principal and auxiliary mechanism reactions specifics are provided in the Appendix B.

2.2 Experimental

Overall, 40 experiments (16 characterization runs and 24 isoprene runs) were conducted in the UNC Dual gas-phase chamber (Pittsboro,NC). Sixteen characterization runs were chosen to evaluate the light model and wall chemistry parameters represented in the auxiliary mechanism [25]. Species in these runs include carbon monoxide (CO), methane (CH_4), ethene (C_2H4) and formaldehyde (HCHO). These are explicit species in the chemical mechanism and whose kinetic information is well quantified. These runs are outlined in Table 1.

Table 1 Characterization Runs – Initial concentration.

Date/side	Compound injected	Injection (ppm)	Initial NO_X(ppm)	Initial NO (ppm)	Initial NO2 (ppm)
OC0984BLUE	HCHO	0.96	0.5	0.35	0.15
ST3097RED	HCHO	2	0.32	0.27	0.05
ST2396RED	HCHO	0.5	0.33	0.28	0.05
ST2396BLUE	HCHO	1	0.33	0.28	0.05
JL1588RED	HCHO	0.79	0.31	0.22	0.09
JL1588BLUE	HCHO	0.43	0.3	0.21	0.09
AU2497RED	ETHE	1.92	0.32	0.29	0.03
AU2497BLUE	ETHE	1.84	0.32	0.29	0.03
AU2393BLUE	ETHE	0.49	0.33	0.28	0.05
AU1688BLUE	ETHE	0.97	0.41	0.34	0.07
AU1092RED	CH_4	500	0.35	0.28	0.07

AU1092BLUE	CH_4	250	0.35	0.28	0.07
AU0197RED	CH_4	500	0.35	0.3	0.05
AU0197BLUE	CH_4	250	0.34	0.29	0.05
ST3097BLUE	CO	250	0.33	0.28	0.05
AU3093BLUE	CO	100	0.32	0.28	0.04

Note: Dates/sides trailing code 'RED ' and 'BLUE' denote the side of Dual chamber where the experiment was operated.

Twenty-four isoprene photo-oxidation experiments were also used and shown in Table 2. In this study, runs in which the isoprene:NO_x concentrations have a ratio less than 1.25 (ppm/ppm) were arbitrarily classified as having a low VOC:NO_X ratio or a high NO_X experiment, while those over 1.25 were considered to have a high VOC:NO_X ratio or a lower NO_X experiment.

Table 2 Isoprene Runs – Initial injected species and concentration

Date/Side	ISOP:NO_X (ppm/ppm)	initial ISOP (ppm)	initial NO_X (ppm)	initial NO (ppm)	initial NO_2 (ppm)
JN1793BLUE	0.18	0.1	0.54	0.47	0.07
JN1793RED	0.35	0.19	0.54	0.47	0.07
JL1780RED	0.44	0.2	0.46	0.36	0.1
JN2381BLUE	0.58	0.26	0.45	0.32	0.13
JL2381RED	0.65	0.28	0.43	0.35	0.08
JN2381RED	1.04	0.46	0.44	0.31	0.13
JL1780BLUE	1.11	0.52	0.47	0.36	0.11
JN2697BLUE	1.13	0.38	0.34	0.27	0.07
JN2592RED	1.61	0.58	0.36	0.31	0.05
OC1596BLUE	1.78	0.58	0.33	0.29	0.04
OC1596RED*	1.84	0.6	0.33	0.28	0.04
AU0897RED	1.89	1.28	0.68	0.59	0.09
AU1597BLUE	1.9	1.58	0.83	0.78	0.06
JN0298BLUE	2.13	1.5	0.7	0.58	0.12
ST0799BLUE	2.31	1.62	0.7	0.69	0.01
ST1199BLUE	2.47	1.5	0.61	0.6	0.01
JN2996RED	2.53	1.02	0.4	0.33	0.07
AU1196BLUE	2.91	0.98	0.34	0.29	0.04
JN2996BLUE	3.12	1.26	0.4	0.34	0.07
ST2496RED	3.2	2.06	0.64	0.57	0.07
JN2592BLUE	3.33	1.2	0.36	0.32	0.04
JN2697RED	3.73	1.29	0.35	0.28	0.07
OC0697RED	4.85	3.12	0.64	0.56	0.08
ST1199RED	9.29	1.56	0.17	0.16	0.01

**: 200 ppm CO also injected*

CHAPTER III: RESULTS AND DISCUSSION

3.1 Model Performance

Simulations of with SAPRC07 and the Xie mechanism were statistically compared with observational data in terms of peak O_3 concentration and NO-NO_2 crossover time derived from temporal concentration profiles of NO, NO_2, O_3 (Figure 3 and Figure 4). The NO-NO_2 crossover time implies how fast a mechanism is converting NO to NO_2 and propagating the autocatalytic process of O_3 production. Ozone peak/maximum value is a direct indicator of regulatory interest as reflected by 8-hour ozone standard in NAAQS. Both indicators are reported in the form of normalized mean bias (NMB) computed using Eqn. 1.

$$NMB = \frac{1}{\mathrm{n}}\sum\frac{simulation - observation}{observation} \times 100\% \quad (1)$$

O_3 Peak

O_3 peak concentration values were plotted against observational values shown in Figure 1. For chamber VOC + NO_X daytime experiments, the observed pattern of O_3 temporal profile changes with relative NO_X abundance. A lower NO_X experiment is often characteristic of two O_3 peaks, of which the second peak is due to photolysis of NO_2 released back from reservoir species like PAN. Here we only display the results of the first morning O_3 peak due to direct ozone photochemistry. Under all conditions the Xie O_3 peak was consistently higher than the peak predicted with SAPROC07 by as much as 22.1%. The difference was most pronounced under high NO_X conditions (Figure 2a). Both mechanisms show consistent over-prediction under lower NO_X conditions as shown in Figure 2b and Table 3. It is important to note that under lower NO_X the Xie mechanism is pushing model performance in the wrong direction increasing bias from 8.91 to 15.84%. There is insufficient number of runs in our high NO_X experiments to conclude a statistically significant difference in the two mechanisms. It is clear that the modifications made to SAPRAC07 have resulted in increasing the magnitude of peak ozone.

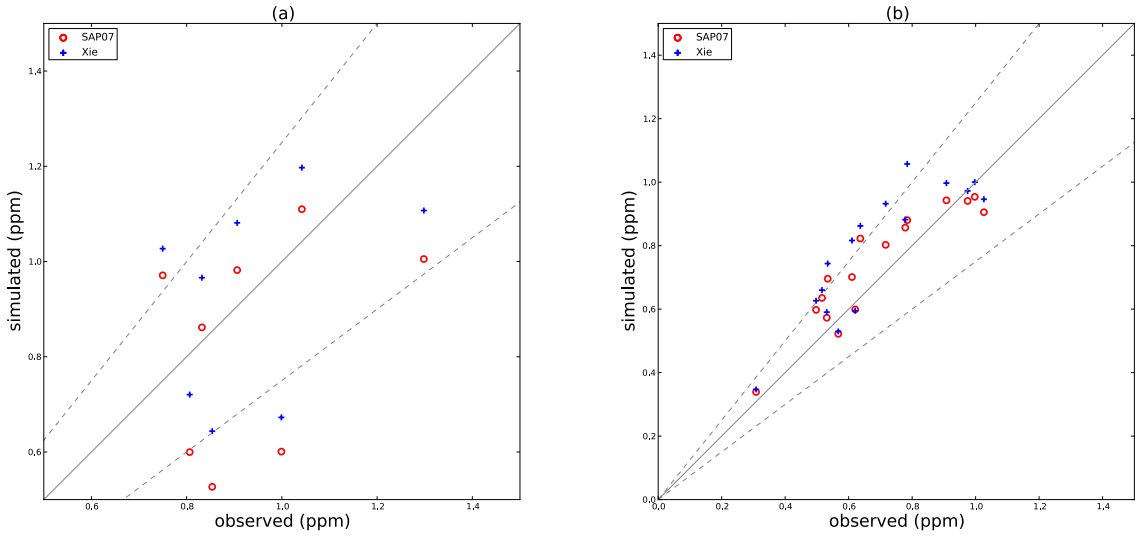

Figure 1 Ozone peak (a) under low ISOP:NO_X ratio and (b) under high ISOP:NO_X ratio
Note: Each point (circle or cross) represents the crossover time of an experiment, with the predicted value on the y axis and measured value on the x axis. The diagonal line suggests perfect modeling agreement with the observation. Red Circle stands for ozone concentration simulated by SAPRC07 and blue cross stands for predictions by the Xie mechanism. The area enclosed by two dashed lines at ±25% is the acceptable range of bias.

Table 3 Summary of O_3 peak model performance statistics

Experiment	Condition	Mechanism	NMB (%)	R^2	P value
N=8	High NO_X	SAPRC07	-9.79	0.13	0.38
		Xie	0.58	0.14	0.36
N=16	Low NO_X	SAPRC07	8.91	0.84	5.74e-07
		Xie	15.84	0.74	1.78e-05

NO-NO_2 Crossover

Figure 1 shows the observed NO-NO_2 crossover time versus simulated results across 8 high NO_X experiments and 16 lower NO_X experiments. We found that both mechanisms under-predict NO-NO_2 crossover time for lower NO_X experiments. The Xie mechanism always had a sooner crossover time than SAPRC07 and was even sooner for lower NO_X experiments. Overall, SAPRC07 over-predicts for 3 out of 24 experiments while Xie only over-predicts one experiment. Detailed statistical results are summarized in Table 4.

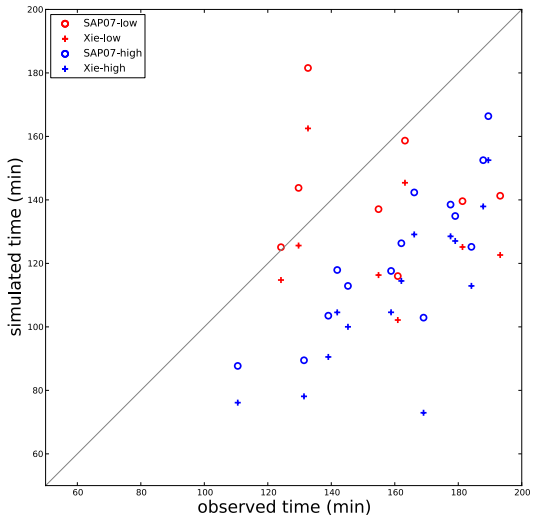

Figure 2 NO-NO2 Crossover time

Note: Circle stands for crossover time simulated by SAPRC07 and cross stands for times predicted by the Xie mechanism. Each point (circle or cross) represents the crossover time of an experiment, with the predicted value on the y axis and measured value on the x axis. The diagonal line suggests perfect modeling agreement with the observation. Red indicates the experiments with low initial ISOP:NO_X and blue for high ISOP:NO_X. Note that the time shown here is the crossover time relative to the start of the experiment.

Table 4 Summary of crossover time statistics

Experiment	Condition	Mechanism	NMB (%)	R^2
N=8	High NO_X	SAPRC07	-5.4	0.022
		Xie	-16.0	0.032
N=16	Low NO_X	SAPRC07	-24.1	0.77
		Xie	-32.3	0.68

3.2 Process Analysis

In the following analysis, our focus shifts from model-to-observation comparison to mechanism inter-comparison under different initial ISOP:NO_X ratios. Chemical reaction process analysis is applied in this step using PERMM (Python-based Environment for Reaction Mechanisms/Mathematics) [26]. Process analysis is based on the concepts of integrated reaction rate (IRR) analysis[27],[28]. The IRR over each time step of each reaction in the mechanism is outputted to .irr file and the IRR over the course of the simulation and its corresponding reaction is outputted to .irrmg file by MORPHO. PERMM reads in these MORPHO outputs and provides an interface to obtain net reactions and quantify radical and NOx budgets. To account for the pattern observed in model performance assessment, we conducted reaction process analysis on two selected cases -- one high NOx case and one lower NOx case (Table 5). The difference between SAPRC07 and Xie is reported in the form of relative difference (RD) using Eqn. 2. In this case, a positive RD value would suggest Xie has a higher cycle number, vice versa.

$$RD = \frac{Xie - SAPRC07}{SAPRC07} \times 100\% \quad (2)$$

Case Study

The concentration profiles of O_3, NO_X, and isoprene are displayed side by side in Figure 3 and Figure 4. Ozone temporal concentration profiles are characteristic of distinctive observed patterns under different initial VOC and NOx concentration levels. For a typical high NO_X (low VOC:NO_X ratio) chamber experiment (Figure 3a), the system runs out of NO late in the day compared with the lower NO_X (high VOC:NOx ratio) experiment and gradually makes ozone until 5 pm for our high NO_X experiment JN2381BLUE..In comparison, a typical lower NO_X experiment has a shorter-lasting photochemical production of ozone. For example for our Low NO_X experiment JN2697RED, the second O_3 peak (0.75 ppb) occurs at 2 pm due to NO_2 released from its reservoir species NOz.

Table 5 Selected study Cases Initial Condition and O_3 peak concentration

Experiment	Initial ISOP:NO_X (ppm/ppm)	Initial isoprene (ppm)	Initial NO_X (ppm)	O3 peak (ppm)	O3 max (ppm)
JN2381BLUE	0.58	0.26	0.45	0.85	0.85
JN2697RED	3.73	1.29	0.35	0.57	0.75

Note: Here only the measured values of the first ozone peak are shown.

For JN2381BLUE (high NO_X), both mechanisms under-predict the NO-NO_2 crossover time and maximum O_3 concentration. Neither mechanism is able to predict the actual O_3 peak around 5 pm. The Xie mechanism had a result closer to the measurement. For JN2697RED (lower NO_X), both mechanisms over-predict the NO-NO_2 crossover time and under-predict the morning O_3 peak to a similar extent. The Xie mechanism, however, produces O_3 faster in the afternoon increasing final O_3 concentrations by 0.21 ppb and 0.35 ppb compared to the observation and SAPRC07. Regardless of the difference of the ability to reproduce observations the Xie mechanism predicts an earlier crossover time and a higher O_3 peak concentration and is visually represented in Figure 3. Table 6 lists the reactions for the OH reaction with

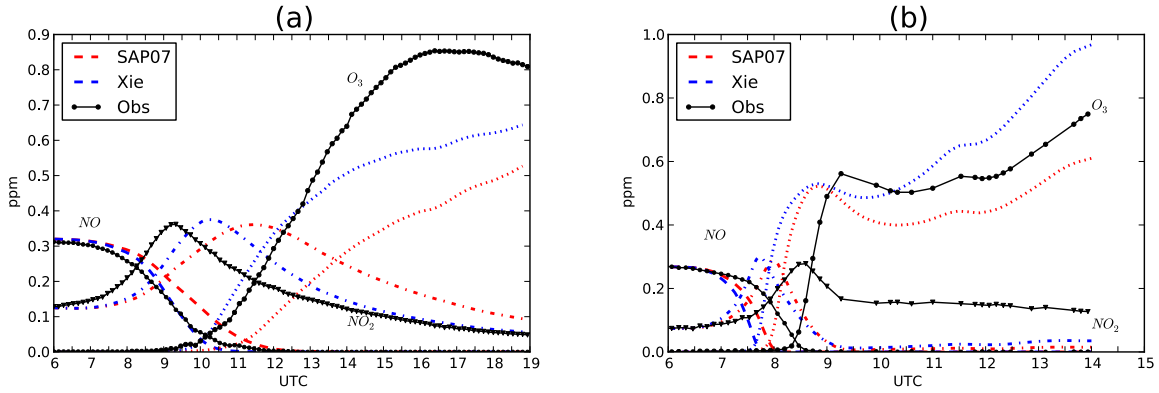

Figure 3 Ozone and NO_X concentration time profile for: (a) JN2381BLUE (High NOx) and (b) JN2697RED (Lower NOx)
Note: Observation values are plotted in black with measured data points. Simulation by SAPRC07 is plotted in red and Xie in blue. "SAP07" stands for SAPRC07 and "Obs" stands for observation.

isoprene and its resulting products. Figure 4 shows the isoprene decay for the two experiments with the Xie mechanism oxidizing more isoprene faster. The loss of isoprene due to the reaction with OH is consistent with the OH concentration levels shown in Figure 5. Because of that, the first generated ISOPO2 of the Xie mechanism dominates over RO2C (SAPRC07) in NO-to-NO2 conversion, and produces more formaldehyde (HCHO) and HO2. There was up to a three times increase in HO2 production rate from aldehyde photolysis, most of which is from formaldehyde (Figure 7). HO_2 from

aldehyde converts NO to NO2 and produces a OH radical. This OH will participate in a new round of VOC oxidation and propagation reactions, thus amplifying the entire chain. Accordingly, more OH is predicted by the Xie mechanism as shown in Figure 5. The increased OH production permits the Xie mechanism to continue to oxidize VOCs until the end of the experiment (Figure 6).

Table 6 The initial steps of isoprene oxidation by OH for the SAPRC07 and Xie mechanisms

Mechanism	Reactions	Rate
SAPRC07	ISOP + OH = 0.986***RO2C** + 0.093*RO2XC + 0.093*zRNO3 + 0.907*xHO2 + 0.624*xHCHO+ 0.23*xMACR + 0.32*xMVK + 0.357*xIPRD + yR6OOH + 0.167*XC	k[BE06]
	xHO2 + NO = HO2 + NO	k[BR07]
	RO2C + NO ----> NO2	k[BR07]
Xie	ISOP + OH = **ISOPO2** + ISOPRXN	k[BE06]
	ISOPO2 + NO = 0.40*MVK + 0.26*MACR + 0.883*NO2 + 0.07*ISOPND + 0.047*ISOPNB + **0.66*HCHO** + 0.10*HC5 + 0.043*ARO2 + 0.08*DIBOO + 0.803*HO2	k[BR07]

Note: Rate constant IDs are provided here and their values can be found in Appendix X.

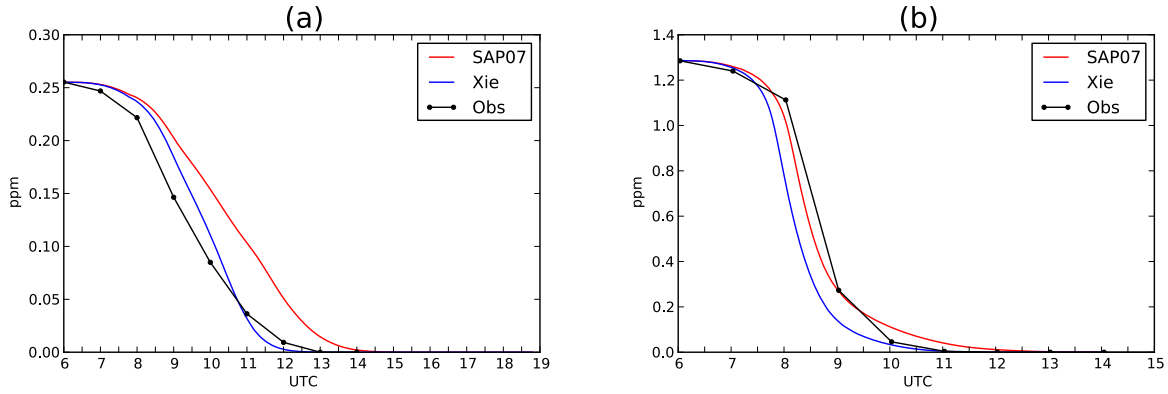

Figure 4 Isoprene concentration time profile for: (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X)
Note: Observation values are plotted in black with measured data points. Simulation by SAPRC07 is plotted in red and Xie in blue.

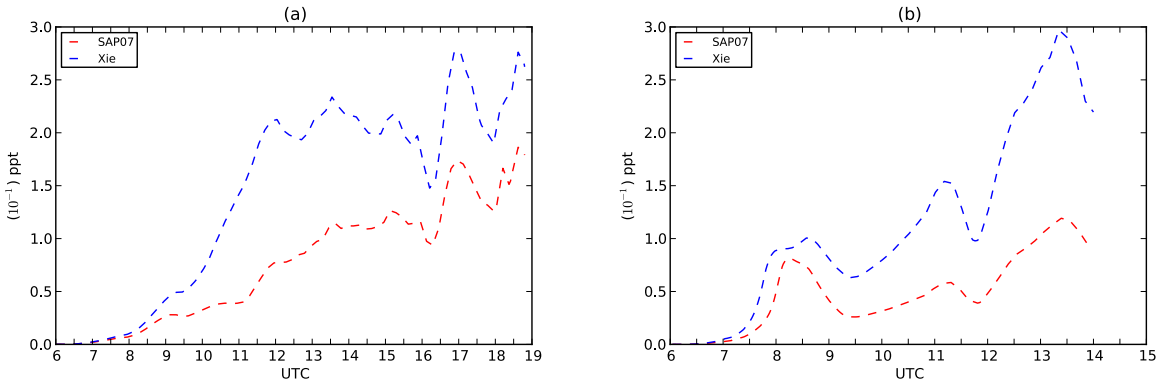

Figure 5 OH concentration time profile for: (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X)

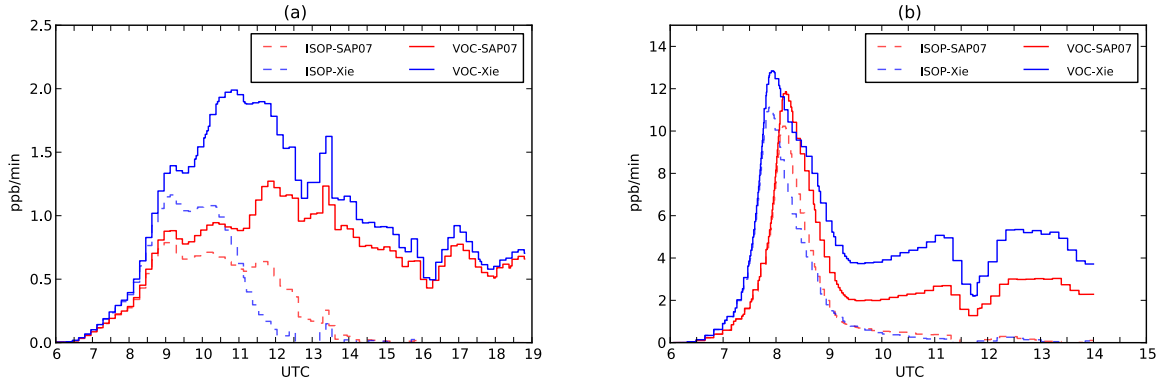

Figure 6 VOCs and isoprene reaction rate against OH time series for: (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X)

Note: VOCs reaction rate is plotted in solid steps and isoprene reaction rate is plotted in dashed steps. Values of SAPRC07 are drawn in red and those of Xie are drawn in blue.

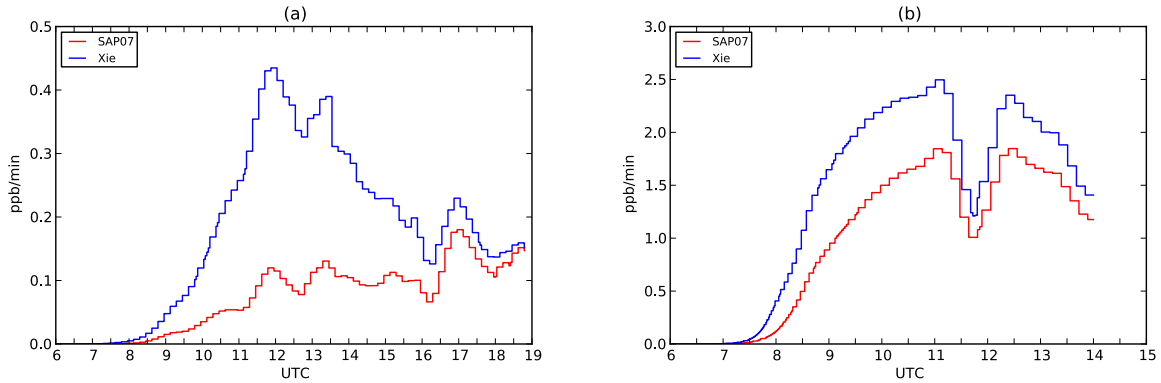

Figure 7 HO_2 production rate from aldehyde time series for: (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X)

Note: For SAPRC07 aldehyde includes formaldehyde (HCHO), acetaldehyde (CCHO) and lumped aldehyde (RCHO). Except for those three aldehyde species in SAPRC07, another two are added in Xie mechanism: glycoaldehyde (HOCCHO) and hydroperoxy aldehydes (HPALD).

Figure 8 shows the integrated reaction rate of VOC + OH (solid lines in Figure 6) over the entire courses of two experiments. Xie mechanism has more OH+VOC reactions due to both the introduction of new species

and the increased reaction of existing species. A complete lists of VOCs reacted with OH are shown in their own identities in

Figure 9. Note that there is a mass shift within certain species because of changed pathways in Xie mechanism. For example, RNO3 are now represented by species including ISOPND, ISOPNB, NIT1, NISOP2OOH, MACRN, MVKN, and ETHLN, RNO3I and itself in the Xie mechanism. So part of the OH radicals that used to react with RNO3 are now distributed to reaction with each of those species.

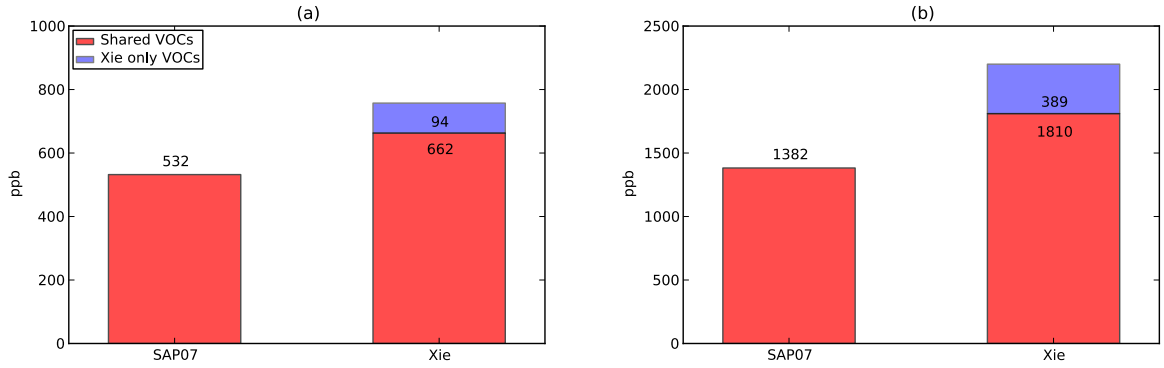

Figure 8 Comparison of Total OH+VOC reactions IRR: (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X)
Note: Total amount of VOCs reacting with OH is plotted in separate bars. Red denotes the VOCs that the two mechanisms share during the course of the simulations; blue denotes the VOCs that only react in the Xie's simulations.

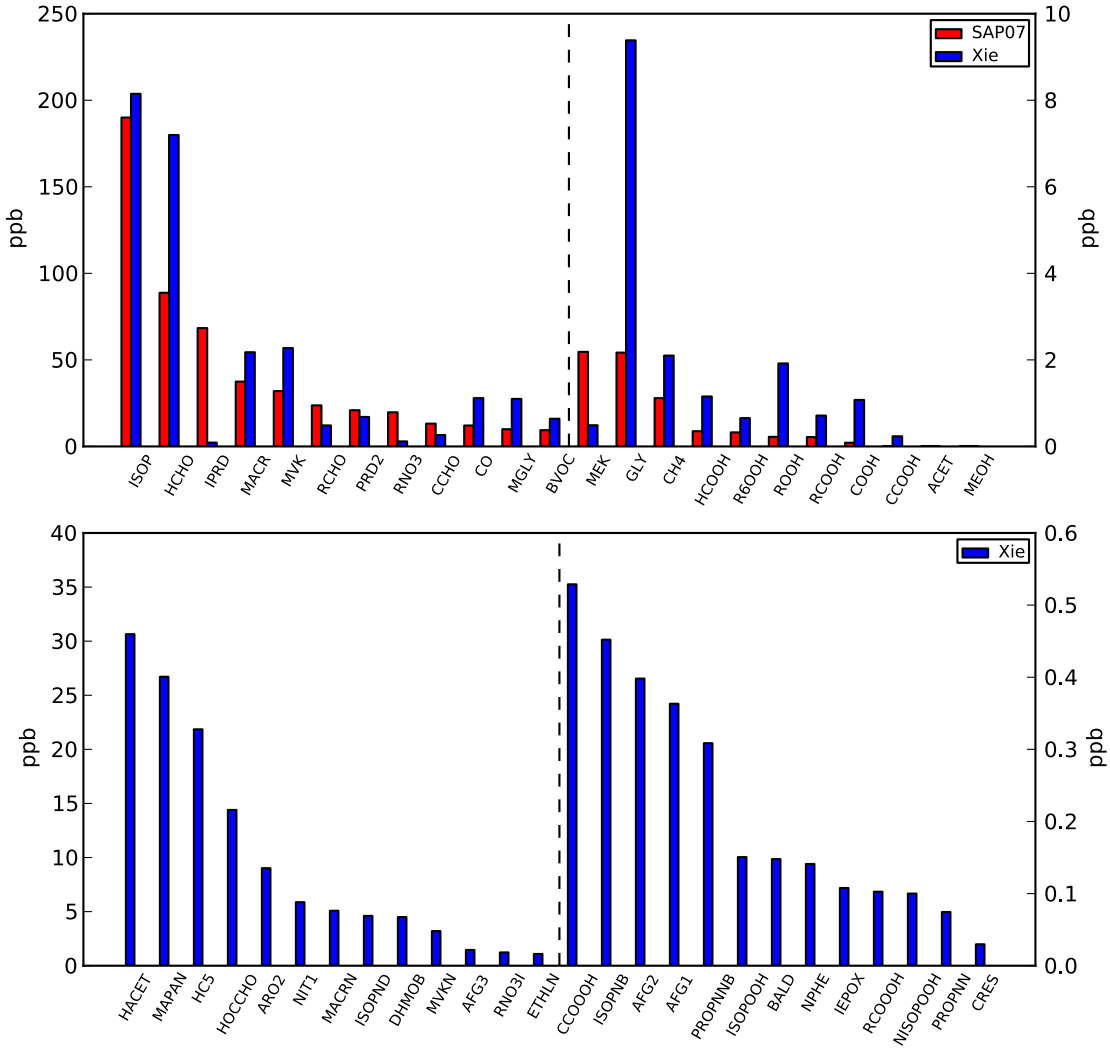

Figure 9 Detailed comparison of mass through various VOC+OH reaction pathways for JN2381BLUE (High NO_X)

Note: Each VOC reacting with OH is plotted in separate bars. The upper plot contains the VOCs that two mechanisms share and have actual mass flow during the course of the simulations; the bottom plot contains the VOCs that have mass flow only in the simulations by Xie mechanism. Right axis is for species right to the vertical dashed line.

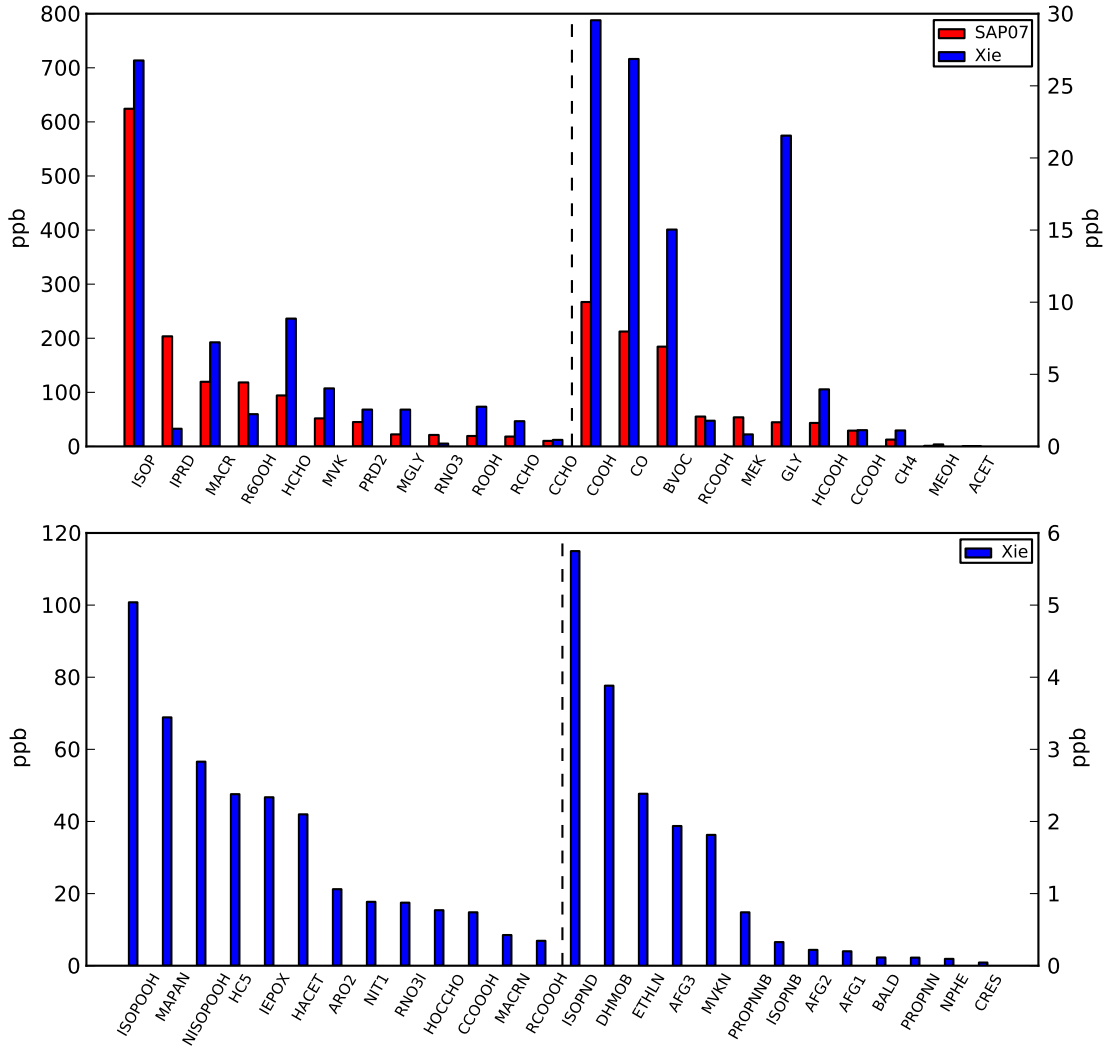

Figure 10 Detailed comparison of mass through various VOC+OH reaction pathways for JN2697RED (Lower NO_X)

Note: Each VOC reacting with OH is plotted in separate bars. The upper plot contains the VOCs that two mechanisms share and have actual mass flow during the course of the simulations; the bottom plot contains the VOCs that have mass flow only in the simulations by Xie mechanism. Right axis is for species right to the vertical dashed line.

A summary of the OH radical budget is tabulated in Table 7. This OH cycle number is an indication of the efficiency of the system in using OH radicals. In the simulations by the Xie mechanism, OH cycle is about -29.3% different in the high NO_X case, but 8% different in the lower NO_X case. In the high NO_X case, the Xie mechanism was less efficient in use of OH even though it produced twice the amount of new OH (Table 7). The increased OH concentration in this experiment, coupled with higher NO_2 concentrations, increased the competition of OH through termination reaction (R 6) instead of VOC + OH reactions. For the lower NO_X case, this termination pathway is not as significant so the difference in OH cycle for the two mechanisms is less.

$$NO_2 + OH \rightarrow HNO_3 \qquad (R\ 6)$$

Table 7 OH radical budget for: (Upper Row) JN2381BLUE (High NO_X) and (Lower Row) JN2697RED (Lower NO_X) experiments.

Experiment	Mechanism	New OH (ppb)			OH + VOC (ppb)	OH + NO2 (ppb)	OH cycle (unitless)
		Inorganic	Organic	Total			
JN2381BLUE	SAPRC07	29.4	56.2	85.5	532	140.9	8.2
	SAPRC07Xie	34.3	136.8	171.2	756	210.3	5.8
JN2697RED	SAPRC07	46.5	476.2	522.7	1382	13.9	2.5
	SAPRC07Xie	67.6	670.4	738	2199	30.8	2.7

The photolysis of NO_2 is the dominant pathway to make O_3 in the troposphere. Table 8 shows that the reactions of NO with XO2 and NO_Z account for over 50% of NO_2 production in the Xie mechanism compared to 35% in SAPRC07. The remaining 49% of NO_2 comes from reaction of NO with O_3 in the Xie mechanism, compared to 65% in SAPRC07. Therefore, the Xie mechanism is able to produce more O_3. For the lower NO_X case, there is 59% difference for the second peak O_3 concentration. Table 8 shows that about 50% more NO_2 is recycled from NO_Z in the Xie mechanism than in SAPRC07, causing this increase in ozone production. Table 9 shows the NO cycles for both experiments. In high NO_X experiments, the increased nitrogen termination reactions result in a 20% decrease in the NO cycle. In lower NO_X experiments, the reconstruction of the isoprene oxidation pathways in Xie producing NO_2 from NO_Z species result in an increasing rate of NO_2 production in the afternoon (Figure 12 b), and therefore a higher NO cycle. In this experiment, the NO cycle difference between two mechanisms is the largest (32%) among all experiments. This is the reason for the sustained ozone production, resulting in the

increasing O_3 concentrations shown in Figure 3. The consistency remains for experiments having higher ISOP:NO_X ratios, of which the second peak differences between two mechanisms are even larger.

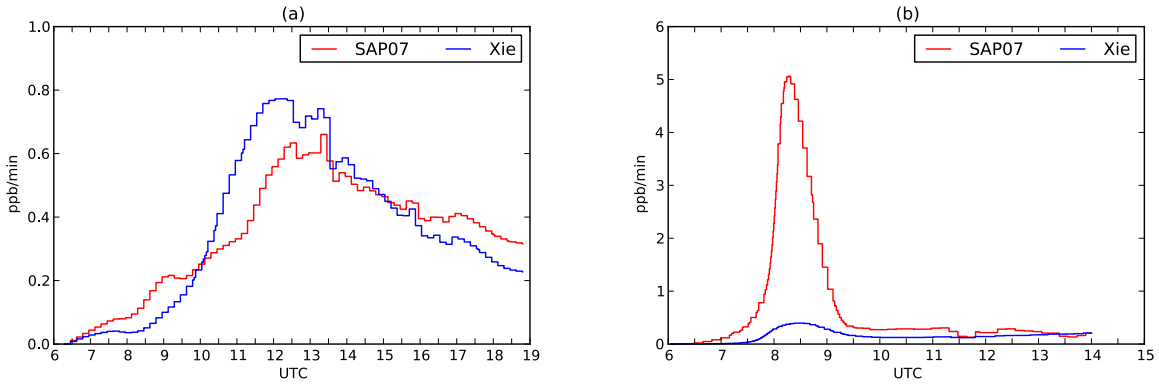

Figure 11 Nitrogen loss reaction rate time series through deposition of HNO_3 and nitrogen loss (XN): (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X).

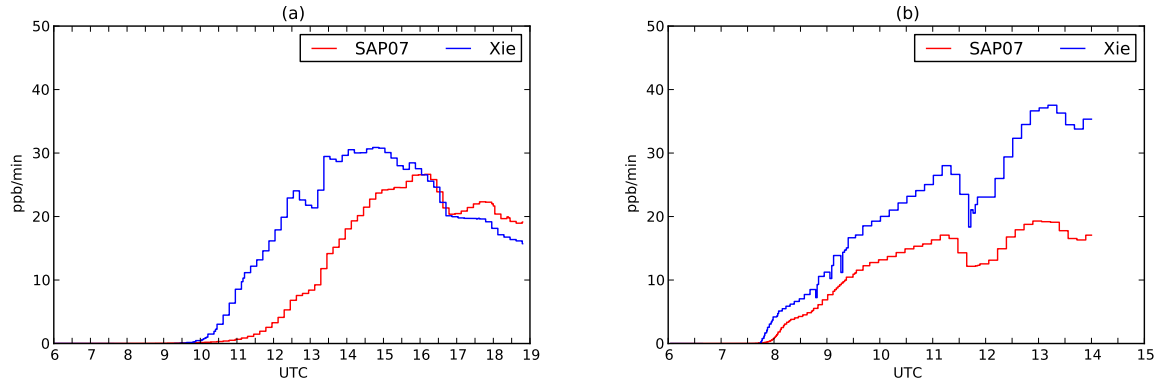

Figure 12 NO_X recycling rate time series from oxidized form NO_2: (a) JN2381BLUE (High NO_X) and (b) JN2697RED (Lower NO_X).

Table 8 NO_2 production irr (ppb) from NO conversion and recycling from NO_Z: (Upper Row) JN2381BLUE (High NO_X) and (Lower Row) JN2697RED (Lower NO_X)

Experiment	Mechanism	NO->NO_2 (ppb)				NO_Z -> NO_2 (ppb)	Total NO_2 (ppb)
		NO+XO2	NO+NO3	NO+O3	Total		
JN2381 BLUE	SAP07	1191	1442	27575	30208	12061	42269
	Xie	1449	1479	20991	23920	18301	42221
JN2697 RED	SAP07	2138	93	4537	6721	9686	16407
	Xie	2790	336	5901	8860	17180	26040

Note: NO to NO2 conversion include conversion by XO2 (Ξ HO2 + RO2), NO3 and O3.

Table 9 NO cycle calculation specifics: (Upper Row) JN2381BLUE (High NO_X) and (Lower Row) JN2697RED (Lower NO_X)

Experiment	Mechanism	New NO (ppb)				NO -> NO2 (ppb)	NO cycle (unitless)
		Injection	HONO	WHNO3	Total		
JN2381BLUE	SAPRC07	445	8	4	457	30208	66.1
	SAPRC07Xie	445	8	4	457	23920	52.4
JN2697RED	SAPRC07	342	1	0	343	6721	19.6
	SAPRC07Xie	342	1	0	343	8860	25.9

Note: NO cycle number = amount of NO to NO2 conversion/new NO.

We found that the majority of NO_2 recycling increase comes from PANs (Figure 13). Xie mechanism predicts 64% more NO_2 from PANs (PAN, MAPAN & PAN2) than SAPRC07 and that increase accounts for 85% of the total increase in NO_2 recycling. This is due to increased first-generation VOCs products and NO_2 concentration, thus more PANs being made. The Xie mechanism has changed the radical balance of SAPRC07 and directed more NO_X to its temporary reservoir species instead of terminating it through XN (Figure 11b).

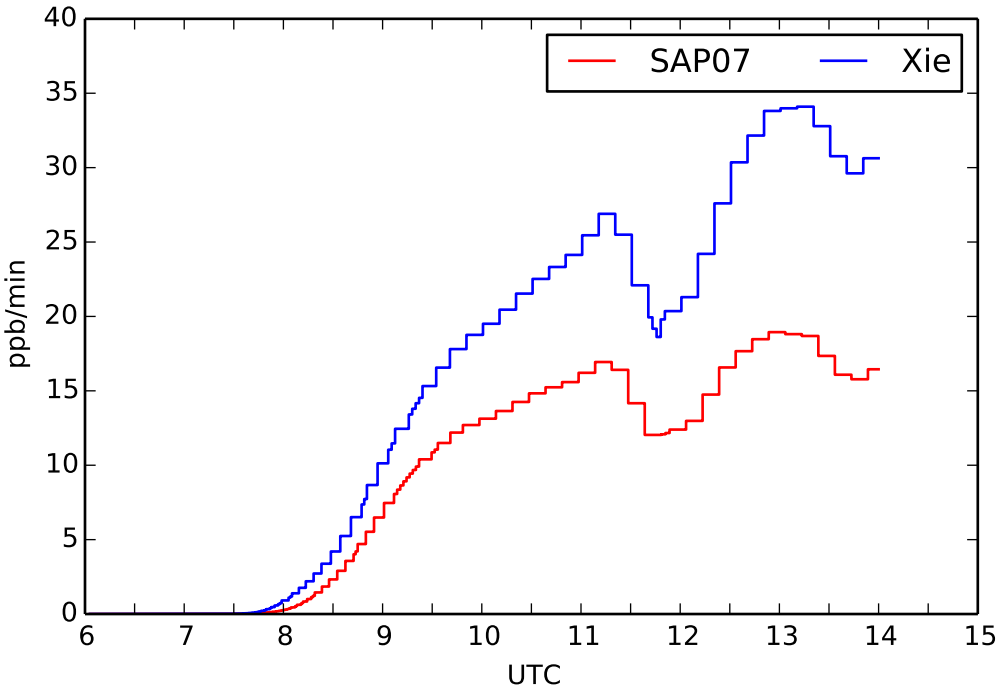

Figure 13 NO_2 recycling rate from PANs for JN2697RED (Lower NO_X).

Figure 14 shows the percent difference between the two mechanisms of the OH and NO cycle for the entire experimental set. In the high NOX experiments, the difference in OH cycle is smaller than that in the lower NO_X experiments. When the experimental conditions are at lower NO_X concentrations, the Xie mechanism tends to have a higher OH cycle. A similar trend is observed in NO cycle difference (Figure 14b). The Xie mechanism has the ability to produce more OH attack on VOCs and convert more NO to NO_2 than the SAPRAC07 mechanism. Under high NO_X conditions, this results in higher NO_2 and OH concentrations and thus increased termination reactions. Although more NO_2 and ultimately O_3 are produced, the OH and NO cycle are lowered. In the lower NO_X experiments, the termination reactions are not as large and the recycled NO_2 late in the day accounts for the differences in the cycle numbers with the SAPRAC07 mechanism.

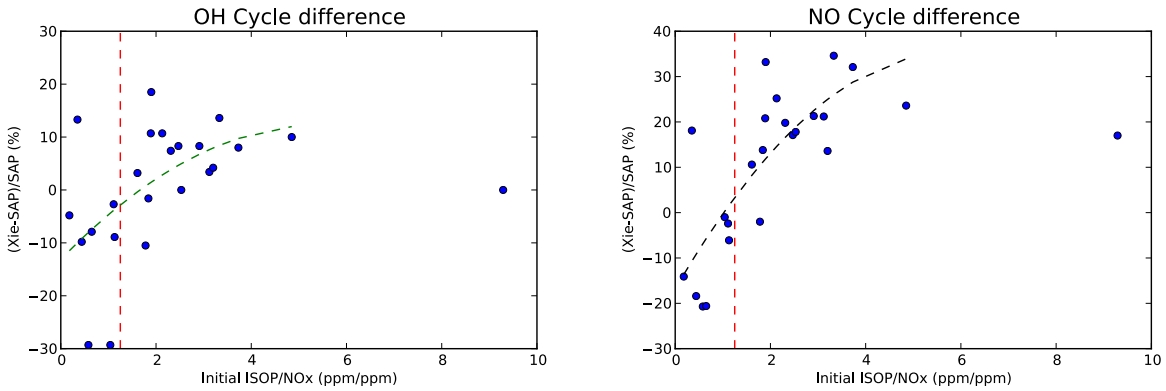

Figure 14 Radical cycle relative difference with regard to initial isoprene:NO_X ratios: (L) OH cycle (R) NO cycle

Note: Each blue point stands for an experiment. The vertical red dashed lines separate the high NOX on the left and low NOX experiments on the right. The dashed green trendlines are for visual aids only. A positive value means Xie mechanism has a higher cycle number, vice versa.

Sensitivity Runs

Model performance results under lower NO_X conditions prompted several sensitivity runs exploring low NO_X chemistry and NO_2 recycling. Again, the lower NO_X experiment selected for process analysis JN2697RED will be used as our testing case. Recent chamber experimental work by Fuchs et al. (2013) confirmed OH regeneration from HPALD produced in ISOPO2 unimolecular reactions (1,6-H shift) but the rate constant $k_{1,6\text{-isom}} = 8.5 \times 10^8 \exp(-5930/T)$ cm^3/s in Leuven isoprene mechanism (LIM) [29] is too large. They evaluated against isoprene photo-oxidation experiments the values of $k_{1,6\text{-isom}}$ and proposed a rate of $6.20 \times 10^8 \exp(-7700/T)$ cm^3/s that can reproduced observed OH [30]. However, their experiments were not able to give a more accurate quantification of $k_{1,6\text{-isom}}$ because of uncertainties in

rate coefficient value for 1,5-H shift isomerization of ISOPO2 and additional recycling of unknown peroxy radicals. Xie used 4.07×10^8 exp(-7694/T) cm^3/s [31],[32]. Here we simulated with a value of 2.35×10^8 exp(-7694/T) cm^3/s. The second analysis will focus on changing the isoprene nitrates (ISOPN) yield. The original value used in Xie et al.'s paper (2013) is 12%. The value in the CMAQ files Dr. Xie provided was reduced to 6% and we used this value in our simulations so far. Here we zeroed it out to evaluate its effect on NO_2 recycling of the lower NO_X case. The sensitivity parameters and their values are summarized in Table 10.

Table 10 Parameters for sensitivity analysis

Case	Description	ISOPO2 isomerization rate constant	ISOPN yields
Run	BASE	K*	0.06
Run A	Lower $k_{1,6\text{-isom}}$	0.5K	0.06
Run B	Zero ISOPN yield	K	0

**K = 4.07 × 108 exp(-7694/T) cm3/s. BASE is run*

In Run A, halved ISOPO2 isomerization rate constant has no impact on NO-NO_2 crossover time and ozone maximum concentration (1.0% less). In Run B, the shut-off of ISOPN yield from ISOPO2 + NO pathway reduced ozone maximum by 5.5%. This confirms the key role of PANs has played in NO_2 recycling efficiency changes under lower NO_X experiments.

Chapter IV: Conclusion

We evaluated the CMAQ version of SAPRC07 mechanism with improved isoprene oxidation pathways by Xie et al. (2013) against outdoor chamber experiments and the base mechanism SAPRC07. Our model performance results suggest that the Xie mechanism produces more O_3 and predicts a faster NO to NO_2 crossover time than SAPRAC07 for all experiments. Under lower NO_X conditions, both mechanisms over predict observations and the Xie mechanism worsens performance and increases the bias from 8.9% to 15.8%. The Xie mechanism reacts more VOCs due to the increased explicit representation of isoprene oxidation products and subsequent OH formation. This increased rate of VOC reactions results in more NO to NO_2 conversions by peroxy radicals and more production of aldehyde. The Xie mechanism also increases NO_2 recycling from NO_Z species, which accounts for the increase in O_3 concentrations in the afternoon for lower NO_X experiments. The increase in NO2 recycling from PANs accounts for 85% of the total increase in NO_2 recycling. Attempts to improve ozone model performance at lower NO_X experiments showed limited influence to the isoprene nitrates yields from ISOPO2 + OH/NO pathway. A shut-off of ISOPN yield merely resulted in a 5% decrease in ozone maximum concentrations. This confirms that changes in NO_2 recycling efficiency should be attributed to increased PANs production, which is a result of increased initial VOC + OH reactions and NO_2 production. These results underline the importance of further efforts in refining the stoichiometry of isoprene oxidation pathways within a condensed mechanism and further lab studies on characterizing the rate constants for those pathways.

APPENDIX A: XIE MODIFICATION OF SAPRC07T REACTIONS LISTING

```
// ********************************************************************************
// *  Modified SAPRC07C Principal Mechanism by Ying Xie at EPA,       *
// *  in Morpho format by Harshal Parikh                               *
// *  Units in: cm^3_molecule^-1_s^-1                                  *
// ********************************************************************************
//
// Created By:
//  William P. L. Carter
//  CE-CERT
//  University of California Riverside
//  Riverside CA 92521
//  (909) 781-5797, FAX (909) 781-5790
//  carter@cert.ucr.edu
//
//  SAPRC-07 (version C) As used or documented in the following
//  reports or publications:
//
//  Carter, W. P. L. (2010):
//  "Development of the SAPRC-07 Chemical Mechanism and Updated
//   Ozone Reactivity Scales," final report to California Air
//   Resources Board Contracts No. 03-318, 06-408, and 07-730,
//  January 27, 2010
//  (This report can be downloaded via
//   http://www.engr.ucr.edu/~carter/SAPRC/saprc07.pdf)
//
// UNC CHANGES
//
//  Last modified 9/03/10  Harshal, cvt from Carter's text.
//  Last modified November 27, 2010 HEJ re-order rxns, rename JRates
//  Last modified 2/17/12 REJ from mech_SAPRC07TC_AE5_AQ_isoprene_v4_Sep_11.txt
//  Last modified 3/12/14 YC add R[IS137]back; @100*j[MACR_to_RO2]
//  Last modified 3/17/14 YC add jrates of HPALD and NOA
//
// Notes:
// 1. Changed photolysis rate names to `UNC STD` for use with JTableConfig.yaml
//
// Needed photolysis rates:
//   NO2_to_O3P
//   O3_to_O3P
//   O3_to_O1D
//   NO3_to_NO
//   NO3_to_NO2
// xxxx N2O5_to_NO2
//   HONO_to_OH
//   HNO3_to_OH
//   PNA_to_HO2
//   H2O2_to_OH
//
//   HCHO_to_HO2
//   HCHO_to_H2
//   CCHO_to_HO2
//   C2CHO_to_HO2
//
```

```
//   ACRO_to_RO2
//   MACR_to_RO2
//   BzCO_to_NR
//
//   COC_to_RO2
//   MEK_to_RO2
//   MVK_to_RO2
//
//   GLY_to_HO2
//   GLY_to_CO
//   MGLY_to_HO2
//   CCOCOC_to_RO2
//   AFG1_to_RO2
//
//   COOH_to_HO2
//
//   IC3ONO2_to_NO2
//   PAN_to_NO2
//
//   HPALD_to_Prds
//   NOA_to_Prds
//
// 2. Need to implement Carter's `computed rates` for the large number of xPROD
//      See pdf page 170 of SAPRAC07 report (labeled page 155).
//

NAMES
 IgnSpcIDs += { XC, XN } ;

NAMES
 PhotoRateIDs += {NO2_to_O3P};
R[I1]= NO2 -hv-> NO + O3P    @ j[NO2_to_O3P] ;
// Absorption coefficients and quantum yields based on NASA06

R[I2]= O3P + O2 + M ----> O3    @ 5.68e-34*(T_300)^-2.60 ;  // IUPAC06
R[I3]= O3P + O3 ---->          @ 8.00e-12*EXP(-2060.0/TK) ;
R[I4]= O3P + NO ----> NO2    @ TROE( 9.00e-32*(T_300)^-1.50,  3.00e-11, b[M],0.60) ;
R[I5]= O3P + NO2 ----> NO    @ 5.50e-12*EXP(188.0/TK) ;
R[I6]= O3P + NO2 ----> NO3    @ TROE( 2.50e-31*(T_300)^-1.80,  2.20e-11*(T_300)^-0.70, b[M],0.60) ;
R[I7]= O3 + NO ----> NO2    @ 3.00e-12*EXP(-1500.0/TK) ;
R[I8]= O3 + NO2 ----> NO3    @ 1.40e-13*EXP(-2470.0/TK) ;
R[I9]= NO + NO3 ----> 2*NO2    @ 1.80e-11*EXP(110.0/TK) ;
R[I10]= NO + NO + O2 ----> 2*NO2    @ 3.30e-39*EXP(530.0/TK) ;
R[I11]= NO2 + NO3 ----> N2O5    @ TROE( 3.60e-30*(T_300)^-4.10,  1.90e-12*(T_300)^0.20, b[M],0.35) ;
R[I12]= N2O5 ----> NO2 + NO3    @ TROE( 1.30e-03*(T_300)^-3.50*EXP(-11000.0/TK),
9.70e+14*(T_300)^0.10*EXP(-11080.0/TK), b[M],0.35) ;
R[I13]= N2O5 + H2O ----> 2*HNO3    @ 2.50e-22 ;
R[I14]= N2O5 + H2O + H2O ----> 2*HNO3    @ 1.80e-39 ;
R[I15]= NO2 + NO3 ----> NO + NO2    @ 4.50e-14*EXP(-1260.0/TK) ;

NAMES
 PhotoRateIDs += { NO3_to_NO, NO3_to_NO2 };

R[I16]= NO3 -hv-> NO    @ j[NO3_to_NO] ;
R[I17]= NO3 -hv-> NO2 + O3P    @ j[NO3_to_NO2] ;
```

```
NAMES
 PhotoRateIDs += {O3_to_O1D};
R[I18]= O3 -hv-> O1D    @ j[O3_to_O1D] ;

NAMES
 PhotoRateIDs += {O3_to_O3P};

R[I19]= O3 -hv-> O3P    @ j[O3_to_O3P] ;
R[I20]= O1D + H2O ----> 2*OH    @ 1.63e-10*EXP(60.0/TK) ;
R[I21]= O1D + M ----> O3P    @ 2.38e-11*EXP(96.0/TK) ;
R[I22]= OH + NO ----> HONO    @ TROE( 7.00e-31*(T_300)^-2.60,  3.60e-11*(T_300)^-0.10, b[M],0.60) ;

NAMES
 PhotoRateIDs += {HONO_to_OH};
R[I23]= HONO -hv-> OH + NO    @ j[HONO_to_OH] ;
R[I24]= OH + HONO ----> NO2    @ 2.50e-12*EXP(260.0/TK) ;

R[I25]= OH + NO2 ----> HNO3

 #if _KHNO3MOLL_
   // Using rate expression from recent Mollner (2010) paper
                                @ TROE( 1.48E-30*T_300^-3.0,
                                        2.58E-11,
                                        b[M],0.60) ;
 #else
 // Using original rate expression from SAPRC07
                                @ TROE( 1.80e-30*T_300^-3.00,
                                        2.80e-11,
                                        b[M],0.60) ;
 #end


R[I26]= OH + NO3 ----> HO2 + NO2    @ 2.00e-11 ;
R[I27]= OH + HNO3 ----> NO3    @ 2.40e-14*EXP(460.0/TK) + LMHW( 6.50e-34*EXP(1335.0/TK),
2.70e-17*EXP(2199.0/TK), b[M]) ;

NAMES
 PhotoRateIDs += {HNO3_to_OH};
R[I28]= HNO3 -hv-> OH + NO2    @ j[HNO3_to_OH] ;

R[I29]= OH + CO ----> HO2 + CO2    @ ( 1.44e-13*EXP(-0.0/TK) +  3.43e-33*EXP(-0.0/TK)*b[M]) ;
R[I30]= OH + O3 ----> HO2    @ 1.70e-12*EXP(-940.0/TK) ;
R[I31]= HO2 + NO ----> OH + NO2    @ 3.60e-12*EXP(270.0/TK) ;
R[I32]= HO2 + NO2 ----> HNO4    @ TROE( 2.00e-31*(T_300)^-3.40,  2.90e-12*(T_300)^-1.10,
b[M],0.60) ;
R[I33]= HNO4 ----> HO2 + NO2    @ TROE( 3.72e-05*(T_300)^-2.40*EXP(-10650.0/TK),
5.42e+15*(T_300)^-2.30*EXP(-11170.0/TK), b[M],0.60) ;
NAMES
 PhotoRateIDs += {PNA_to_HO2};
R[I34]= HNO4 -hv-> 0.61*HO2 + 0.61*NO2 + 0.39*OH + 0.39*NO3    @ j[PNA_to_HO2] ;
R[I35]= HNO4 + OH ----> NO2    @ 1.30e-12*EXP(380.0/TK) ;
R[I36]= HO2 + O3 ----> OH    @ 2.03e-16*(T_300)^4.57*EXP(693.0/TK) ;
R[I37]= HO2 + HO2 ----> HO2H    @ ( 2.20e-13*EXP(600.0/TK) +  1.90e-33*EXP(980.0/TK)*b[M]) ;
R[I38]= HO2 + HO2 + H2O ----> HO2H    @ ( 3.08e-34*EXP(2800.0/TK) +  2.66e-
54*EXP(3180.0/TK)*b[M]) ;
R[I39]= NO3 + HO2 ----> 0.8*OH + 0.8*NO2 + 0.2*HNO3    @ 4.00e-12 ;
```

```
R[I40]= NO3 + NO3 ----> 2*NO2    @ 8.50e-13*EXP(-2450.0/TK) ;
NAMES
 PhotoRateIDs += {H2O2_to_OH};
R[I41]= HO2H -hv-> 2*OH    @ j[H2O2_to_OH] ;
R[I42]= HO2H + OH ----> HO2    @ 1.80e-12 ;
R[I43]= OH + HO2 ---->          @ 4.80e-11*EXP(250.0/TK) ;
R[I44]= OH + SO2 ----> HO2 + SULF + SULRXN    @ TROE( 3.30e-31*(T_300)^-4.30,  1.60e-12,
b[M],0.60) ;
R[I45]= OH + H2 ----> HO2    @ 7.70e-12*EXP(-2100.0/TK) ;
R[BR01]= MEO2 + NO ----> NO2 + HCHO + HO2    @ 2.30e-12*EXP(360.0/TK) ;
R[BR02]= MEO2 + HO2 ----> COOH    @ 3.46e-13*(T_300)^0.36*EXP(780.0/TK) ;
R[BR03]= MEO2 + HO2 ----> HCHO    @ 3.34e-14*(T_300)^-3.53*EXP(780.0/TK) ;
R[BR04]= MEO2 + NO3 ----> HCHO + HO2 + NO2    @ 1.30e-12 ;
R[BR05]= MEO2 + MEO2 ----> MEOH + HCHO    @ 6.39e-14*(T_300)^-1.80*EXP(365.0/TK) ;
R[BR06]= MEO2 + MEO2 ----> 2*HCHO + 2*HO2    @ 7.40e-13*EXP(-520.0/TK) ;
R[BR07]= RO2C + NO ----> NO2    @ 2.60e-12*EXP(380.0/TK) ;
R[BR08]= RO2C + HO2 ---->          @ 3.80e-13*EXP(900.0/TK) ;
R[BR09]= RO2C + NO3 ----> NO2    @ 2.30e-12 ;
R[BR10]= RO2C + MEO2 ----> 0.5*HO2 + 0.75*HCHO + 0.25*MEOH    @ 2.00e-13 ;
R[BR11]= RO2C + RO2C ---->          @ 3.50e-14 ;
R[BR12]= RO2XC + NO ----> XN    @ k[BR07] *1.0;
R[BR13]= RO2XC + HO2 ---->          @ k[BR08] *1.0;
R[BR14]= RO2XC + NO3 ----> NO2    @ k[BR09] *1.0;
R[BR15]= RO2XC + MEO2 ----> 0.5*HO2 + 0.75*HCHO + 0.25*MEOH    @ k[BR10] *1.0;
R[BR16]= RO2XC + RO2C ---->          @ k[BR11] *1.0;
R[BR17]= RO2XC + RO2XC ---->          @ k[BR11] *1.0;
R[BR18]= MECO3 + NO2 ----> PAN    @ TROE( 2.70e-28*(T_300)^-7.10,  1.21e-11*(T_300)^-0.90,
b[M],0.30) ;
R[BR19]= PAN ----> MECO3 + NO2    @ TROE( 4.90e-03*EXP(-12100.0/TK),  4.00e+16*EXP(-
13600.0/TK), b[M],0.30) ;
NAMES
 PhotoRateIDs += {PAN_to_NO2};
R[BR20]= PAN -hv-> 0.6*MECO3 + 0.6*NO2 + 0.4*MEO2 + 0.4*CO2 + 0.4*NO3    @ j[PAN_to_NO2] ;
R[BR21]= MECO3 + NO ----> MEO2 + CO2 + NO2    @ 7.50e-12*EXP(290.0/TK) ;
R[BR22]= MECO3 + HO2 ----> 0.7*CCOOOH + 0.3*CCOOH + 0.3*O3    @ 5.20e-13*EXP(980.0/TK) ;
R[BR23]= MECO3 + NO3 ----> MEO2 + CO2 + NO2    @ k[BR09] *1.0;
R[BR24]= MECO3 + MEO2 ----> 0.1*CCOOH + 0.1*HCHO + 0.9*HCHO + 0.9*HO2 + 0.9*MEO2 +
0.9*CO2    @ 2.00e-12*EXP(500.0/TK) ;
R[BR25]= MECO3 + RO2C ----> MEO2 + CO2    @ 4.40e-13*EXP(1070.0/TK) ;
R[BR26]= MECO3 + RO2XC ----> MEO2 + CO2    @ k[BR25] *1.0;
R[BR27]= MECO3 + MECO3 ----> 2*MEO2 + 2*CO2    @ 2.90e-12*EXP(500.0/TK) ;
R[BR28]= RCO3 + NO2 ----> PAN2    @ 1.21e-11*(T_300)^-1.07*EXP(-0.0/TK) ;
R[BR29]= PAN2 ----> RCO3 + NO2    @ 8.30e+16*EXP(-13940.0/TK) ;
R[BR30]= PAN2 -hv-> 0.6*RCO3 + 0.6*NO2 + 0.4*RO2C + 0.4*xHO2 + 0.4*yROOH + 0.4*xCCHO +
0.4*CO2 + 0.4*NO3    @ j[PAN_to_NO2] ;
R[BR31]= RCO3 + NO ----> NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2    @ 6.70e-
12*EXP(340.0/TK) ;
R[BR32]= RCO3 + HO2 ----> 0.75*RCOOOH + 0.25*RCOOH + 0.25*O3    @ k[BR22] *1.0;
R[BR33]= RCO3 + NO3 ----> NO2 + RO2C + xHO2 + yROOH + xCCHO + CO2    @ k[BR09] *1.0;
R[BR34]= RCO3 + MEO2 ----> HCHO + HO2 + RO2C + xHO2 + xCCHO + yROOH + CO2    @ k[BR24]
*1.0;
R[BR35]= RCO3 + RO2C ----> RO2C + xHO2 + xCCHO + yROOH + CO2    @ k[BR25] *1.0;
R[BR36]= RCO3 + RO2XC ----> RO2C + xHO2 + xCCHO + yROOH + CO2    @ k[BR25] *1.0;
R[BR37]= RCO3 + MECO3 ----> 2*CO2 + MEO2 + RO2C + xHO2 + yROOH + xCCHO    @ k[BR27] *1.0;
R[BR38]= RCO3 + RCO3 ----> 2*RO2C + 2*xHO2 + 2*xCCHO + 2*yROOH + 2*CO2    @ k[BR27] *1.0;
R[BR39]= BZCO3 + NO2 ----> PBZN    @ 1.37e-11 ;
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R[BR40]= PBZN ----> BZCO3 + NO2    @ 7.90e+16*EXP(-14000.0/TK) ;
R[BR41]= PBZN -hv-> 0.6*BZCO3 + 0.6*NO2 + 0.4*CO2 + 0.4*BZO + 0.4*RO2C + 0.4*NO3    @
j[PAN_to_NO2] ;
R[BR42]= BZCO3 + NO ----> NO2 + CO2 + BZO + RO2C    @ k[BR31] *1.0;
R[BR43]= BZCO3 + HO2 ----> 0.75*RCOOOH + 0.25*RCOOH + 0.25*O3 + 4*XC    @ k[BR22] *1.0;
R[BR44]= BZCO3 + NO3 ----> NO2 + CO2 + BZO + RO2C    @ k[BR09] *1.0;
R[BR45]= BZCO3 + MEO2 ----> HCHO + HO2 + RO2C + BZO + CO2    @ k[BR24] *1.0;
R[BR46]= BZCO3 + RO2C ----> RO2C + BZO + CO2    @ k[BR25] *1.0;
R[BR47]= BZCO3 + RO2XC ----> RO2C + BZO + CO2    @ k[BR25] *1.0;
R[BR48]= BZCO3 + MECO3 ----> 2*CO2 + MEO2 + BZO + RO2C    @ k[BR27] *1.0;
R[BR49]= BZCO3 + RCO3 ----> 2*CO2 + RO2C + xHO2 + yROOH + xCCHO + BZO + RO2C    @
k[BR27] *1.0;
R[BR50]= BZCO3 + BZCO3 ----> 2*BZO + 2*RO2C + 2*CO2    @ k[BR27] *1.0;
R[BR51]= MACO3 + NO2 ----> MAPAN    @ k[BR28] *1.0;
R[BR52]= MAPAN ----> MACO3 + NO2    @ 1.60e+16*EXP(-13486.0/TK) ;
R[BR53]= MAPAN -hv-> 0.6*MACO3 + 0.6*NO2 + 0.4*CO2 + 0.4*HCHO + 0.4*MECO3 + 0.4*NO3    @
j[PAN_to_NO2] ;
R[BR64]= TBUO + NO2 ----> RNO3 + 0.0*XC    @ 2.40e-11 ;
R[BR65]= TBUO ----> ACETONE + MEO2    @ 7.50e+14*EXP(-8152.0/TK) ;
R[BR66]= BZO + NO2 ----> NPHE    @ 2.30e-11*EXP(150.0/TK) ;
R[BR67]= BZO + HO2 ----> CRES + 0.0*XC    @ k[BR08] *1.0;
R[BR68]= BZO ----> CRES + RO2C + xHO2 + 0.0*XC    @ 1.00e-03 ;
R[R019]= xHO2 + NO ----> NO + HO2    @ k[BR07] *1.0;
R[R020]= xHO2 + HO2 ----> HO2    @ k[BR08] *1.0;
R[R021]= xHO2 + NO3 ----> NO3 + HO2    @ k[BR09] *1.0;
R[R022]= xHO2 + MEO2 ----> MEO2 + 0.5*HO2    @ k[BR10] *1.0;
R[R023]= xHO2 + RO2C ----> RO2C + 0.5*HO2    @ k[BR11] *1.0;
R[R024]= xHO2 + RO2XC ----> RO2XC + 0.5*HO2    @ k[BR11] *1.0;
R[R025]= xHO2 + MECO3 ----> MECO3 + HO2    @ k[BR25] *1.0;
R[R026]= xHO2 + RCO3 ----> RCO3 + HO2    @ k[BR25] *1.0;
R[R027]= xHO2 + BZCO3 ----> BZCO3 + HO2    @ k[BR25] *1.0;
R[R028]= xHO2 + MACO3 ----> MACO3 + HO2    @ k[BR25] *1.0;
R[R029]= xOH + NO ----> NO + OH    @ k[BR07] *1.0;
R[R030]= xOH + HO2 ----> HO2    @ k[BR08] *1.0;
R[R031]= xOH + NO3 ----> NO3 + OH    @ k[BR09] *1.0;
R[R032]= xOH + MEO2 ----> MEO2 + 0.5*OH    @ k[BR10] *1.0;
R[R033]= xOH + RO2C ----> RO2C + 0.5*OH    @ k[BR11] *1.0;
R[R034]= xOH + RO2XC ----> RO2XC + 0.5*OH    @ k[BR11] *1.0;
R[R035]= xOH + MECO3 ----> MECO3 + OH    @ k[BR25] *1.0;
R[R036]= xOH + RCO3 ----> RCO3 + OH    @ k[BR25] *1.0;
R[R037]= xOH + BZCO3 ----> BZCO3 + OH    @ k[BR25] *1.0;
R[R038]= xOH + MACO3 ----> MACO3 + OH    @ k[BR25] *1.0;
R[R039]= xNO2 + NO ----> NO + NO2    @ k[BR07] *1.0;
R[R040]= xNO2 + HO2 ----> HO2 + XN    @ k[BR08] *1.0;
R[R041]= xNO2 + NO3 ----> NO3 + NO2    @ k[BR09] *1.0;
R[R042]= xNO2 + MEO2 ----> MEO2 + 0.5*NO2 + 0.5*XN    @ k[BR10] *1.0;
R[R043]= xNO2 + RO2C ----> RO2C + 0.5*NO2 + 0.5*XN    @ k[BR11] *1.0;
R[R044]= xNO2 + RO2XC ----> RO2XC + 0.5*NO2 + 0.5*XN    @ k[BR11] *1.0;
R[R045]= xNO2 + MECO3 ----> MECO3 + NO2    @ k[BR25] *1.0;
R[R046]= xNO2 + RCO3 ----> RCO3 + NO2    @ k[BR25] *1.0;
R[R047]= xNO2 + BZCO3 ----> BZCO3 + NO2    @ k[BR25] *1.0;
R[R048]= xNO2 + MACO3 ----> MACO3 + NO2    @ k[BR25] *1.0;
R[R049]= xMEO2 + NO ----> NO + MEO2    @ k[BR07] *1.0;
R[R050]= xMEO2 + HO2 ----> HO2 + XC    @ k[BR08] *1.0;
R[R051]= xMEO2 + NO3 ----> NO3 + MEO2    @ k[BR09] *1.0;
R[R052]= xMEO2 + MEO2 ----> MEO2 + 0.5*MEO2 + 0.5*XC    @ k[BR10] *1.0;
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R[R053]= xMEO2 + RO2C ----> RO2C + 0.5*MEO2 + 0.5*XC    @ k[BR11] *1.0;
R[R054]= xMEO2 + RO2XC ----> RO2XC + 0.5*MEO2 + 0.5*XC    @ k[BR11] *1.0;
R[R055]= xMEO2 + MECO3 ----> MECO3 + MEO2    @ k[BR25] *1.0;
R[R056]= xMEO2 + RCO3 ----> RCO3 + MEO2    @ k[BR25] *1.0;
R[R057]= xMEO2 + BZCO3 ----> BZCO3 + MEO2    @ k[BR25] *1.0;
R[R058]= xMEO2 + MACO3 ----> MACO3 + MEO2    @ k[BR25] *1.0;
R[R059]= xMECO3 + NO ----> NO + MECO3    @ k[BR07] *1.0;
R[R060]= xMECO3 + HO2 ----> HO2 + 2*XC    @ k[BR08] *1.0;
R[R061]= xMECO3 + NO3 ----> NO3 + MECO3    @ k[BR09] *1.0;
R[R062]= xMECO3 + MEO2 ----> MEO2 + 0.5*MECO3 + XC    @ k[BR10] *1.0;
R[R063]= xMECO3 + RO2C ----> RO2C + 0.5*MECO3 + XC    @ k[BR11] *1.0;
R[R064]= xMECO3 + RO2XC ----> RO2XC + 0.5*MECO3 + XC    @ k[BR11] *1.0;
R[R065]= xMECO3 + MECO3 ----> MECO3 + MECO3    @ k[BR25] *1.0;
R[R066]= xMECO3 + RCO3 ----> RCO3 + MECO3    @ k[BR25] *1.0;
R[R067]= xMECO3 + BZCO3 ----> BZCO3 + MECO3    @ k[BR25] *1.0;
R[R068]= xMECO3 + MACO3 ----> MACO3 + MECO3    @ k[BR25] *1.0;
R[R069]= xRCO3 + NO ----> NO + RCO3    @ k[BR07] *1.0;
R[R070]= xRCO3 + HO2 ----> HO2 + 3*XC    @ k[BR08] *1.0;
R[R071]= xRCO3 + NO3 ----> NO3 + RCO3    @ k[BR09] *1.0;
R[R072]= xRCO3 + MEO2 ----> MEO2 + 0.5*RCO3 + 1.5*XC    @ k[BR10] *1.0;
R[R073]= xRCO3 + RO2C ----> RO2C + 0.5*RCO3 + 1.5*XC    @ k[BR11] *1.0;
R[R074]= xRCO3 + RO2XC ----> RO2XC + 0.5*RCO3 + 1.5*XC    @ k[BR11] *1.0;
R[R075]= xRCO3 + MECO3 ----> MECO3 + RCO3    @ k[BR25] *1.0;
R[R076]= xRCO3 + RCO3 ----> RCO3 + RCO3    @ k[BR25] *1.0;
R[R077]= xRCO3 + BZCO3 ----> BZCO3 + RCO3    @ k[BR25] *1.0;
R[R078]= xRCO3 + MACO3 ----> MACO3 + RCO3    @ k[BR25] *1.0;
R[R079]= xMACO3 + NO ----> NO + MACO3    @ k[BR07] *1.0;
R[R080]= xMACO3 + HO2 ----> HO2 + 4*XC    @ k[BR08] *1.0;
R[R081]= xMACO3 + NO3 ----> NO3 + MACO3    @ k[BR09] *1.0;
R[R082]= xMACO3 + MEO2 ----> MEO2 + 0.5*MACO3 + 2*XC    @ k[BR10] *1.0;
R[R083]= xMACO3 + RO2C ----> RO2C + 0.5*MACO3 + 2*XC    @ k[BR11] *1.0;
R[R084]= xMACO3 + RO2XC ----> RO2XC + 0.5*MACO3 + 2*XC    @ k[BR11] *1.0;
R[R085]= xMACO3 + MECO3 ----> MECO3 + MACO3    @ k[BR25] *1.0;
R[R086]= xMACO3 + RCO3 ----> RCO3 + MACO3    @ k[BR25] *1.0;
R[R087]= xMACO3 + BZCO3 ----> BZCO3 + MACO3    @ k[BR25] *1.0;
R[R088]= xMACO3 + MACO3 ----> MACO3 + MACO3    @ k[BR25] *1.0;
R[R089]= xTBUO + NO ----> NO + TBUO    @ k[BR07] *1.0;
R[R090]= xTBUO + HO2 ----> HO2 + 4*XC    @ k[BR08] *1.0;
R[R091]= xTBUO + NO3 ----> NO3 + TBUO    @ k[BR09] *1.0;
R[R092]= xTBUO + MEO2 ----> MEO2 + 0.5*TBUO + 2*XC    @ k[BR10] *1.0;
R[R093]= xTBUO + RO2C ----> RO2C + 0.5*TBUO + 2*XC    @ k[BR11] *1.0;
R[R094]= xTBUO + RO2XC ----> RO2XC + 0.5*TBUO + 2*XC    @ k[BR11] *1.0;
R[R095]= xTBUO + MECO3 ----> MECO3 + TBUO    @ k[BR25] *1.0;
R[R096]= xTBUO + RCO3 ----> RCO3 + TBUO    @ k[BR25] *1.0;
R[R097]= xTBUO + BZCO3 ----> BZCO3 + TBUO    @ k[BR25] *1.0;
R[R098]= xTBUO + MACO3 ----> MACO3 + TBUO    @ k[BR25] *1.0;
R[R099]= xCO + NO ----> NO + CO    @ k[BR07] *1.0;
R[R100]= xCO + HO2 ----> HO2 + XC    @ k[BR08] *1.0;
R[R101]= xCO + NO3 ----> NO3 + CO    @ k[BR09] *1.0;
R[R102]= xCO + MEO2 ----> MEO2 + 0.5*CO + 0.5*XC    @ k[BR10] *1.0;
R[R103]= xCO + RO2C ----> RO2C + 0.5*CO + 0.5*XC    @ k[BR11] *1.0;
R[R104]= xCO + RO2XC ----> RO2XC + 0.5*CO + 0.5*XC    @ k[BR11] *1.0;
R[R105]= xCO + MECO3 ----> MECO3 + CO    @ k[BR25] *1.0;
R[R106]= xCO + RCO3 ----> RCO3 + CO    @ k[BR25] *1.0;
R[R107]= xCO + BZCO3 ----> BZCO3 + CO    @ k[BR25] *1.0;
R[R108]= xCO + MACO3 ----> MACO3 + CO    @ k[BR25] *1.0;
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NAMES
 PhotoRateIDs += {HCHO_to_HO2, HCHO_to_H2};
R[BP01]= HCHO -hv-> 2*HO2 + CO    @ j[HCHO_to_HO2] ;
R[BP02]= HCHO -hv-> CO    @ j[HCHO_to_H2] ;
R[BP03]= HCHO + OH ----> HO2 + CO    @ 5.40e-12*EXP(135.0/TK) ;
R[BP07]= HCHO + NO3 ----> HNO3 + HO2 + CO    @ 2.00e-12*EXP(-2431.0/TK) ;
R[BP08]= CCHO + OH ----> MECO3    @ 4.40e-12*EXP(365.0/TK) ;
NAMES
 PhotoRateIDs += {CCHO_to_HO2};
R[BP09]= CCHO -hv-> CO + HO2 + MEO2    @ j[CCHO_to_HO2] ;
R[BP10]= CCHO + NO3 ----> HNO3 + MECO3    @ 1.40e-12*EXP(-1860.0/TK) ;
R[BP11]= RCHO + OH ----> 0.965*RCO3 + 0.035*RO2C + 0.035*xHO2 + 0.035*xCO + 0.035*xCCHO +
0.035*yROOH    @ 5.10e-12*EXP(405.0/TK) ;
NAMES
 PhotoRateIDs += {C2CHO_to_HO2};
R[BP12]= RCHO -hv-> RO2C + xHO2 + yROOH + xCCHO + CO + HO2    @ j[C2CHO_to_HO2] ;
R[BP13]= RCHO + NO3 ----> HNO3 + RCO3    @ 1.40e-12*EXP(-1601.0/TK) ;
R[BP14]= ACETONE + OH ----> RO2C + xMECO3 + xHCHO + yROOH    @ 4.56e-
14*(T_300)^3.65*EXP(429.0/TK) ;
NAMES
 PhotoRateIDs += {COC_to_RO2};
R[BP15]= ACETONE -hv-> 0.62*MECO3 + 1.38*MEO2 + 0.38*CO    @5.00e-1 *  j[COC_to_RO2] ;
R[BP16]= MEK + OH ----> 0.967*RO2C + 0.039*RO2XC + 0.039*zRNO3 + 0.376*xHO2 + 0.51*xMECO3
+ 0.074*xRCO3 + 0.088*xHCHO + 0.504*xCCHO + 0.376*xRCHO + yROOH + 0.3*XC    @ 1.30e-
12*(T_300)^2.00*EXP(-25.0/TK) ;
NAMES
 PhotoRateIDs += {C2COC_to_RO2};
R[BP17]= MEK -hv-> MECO3 + RO2C + xHO2 + xCCHO + yROOH    @1.75e-1 *  j[C2COC_to_RO2] ;
R[BP18]= MEOH + OH ----> HCHO + HO2    @ 2.85e-12*EXP(-345.0/TK) ;
R[BP19]= HCOOH + OH ----> HO2 + CO2    @ 4.50e-13 ;
R[BP20]= CCOOH + OH ----> 0.509*MEO2 + 0.491*RO2C + 0.509*CO2 + 0.491*xHO2 + 0.491*xMGLY
+ 0.491*yROOH + 0.0*XC    @ 4.20e-14*EXP(855.0/TK) ;
R[BP21]= RCOOH + OH ----> RO2C + xHO2 + 0.143*CO2 + 0.142*xCCHO + 0.4*xRCHO +
0.457*xBACL + yROOH + 0.0*XC    @ 1.20e-12 ;
R[BP22]= COOH + OH ----> 0.3*HCHO + 0.3*OH + 0.7*MEO2    @ 3.80e-12*EXP(200.0/TK) ;
NAMES
 PhotoRateIDs += { COOH_to_HO2 };
R[BP23]= COOH -hv-> HCHO + HO2 + OH    @ j[COOH_to_HO2] ;
R[BP24]= ROOH + OH ----> 0.744*OH + 0.251*RO2C + 0.004*RO2XC + 0.004*zRNO3 + 0.744*RCHO +
0.239*xHO2 + 0.012*xOH + 0.012*xHCHO + 0.012*xCCHO + 0.205*xRCHO + 0.034*xPROD2 +
0.256*yROOH + 0.0*XC    @ 2.50e-11 ;

R[BP25]= ROOH -hv-> RCHO + HO2 + OH    @ j[COOH_to_HO2] ;
R[BP26]= R6OOH + OH ----> 0.84*OH + 0.222*RO2C + 0.029*RO2XC + 0.029*zRNO3 + 0.84*PRD2 +
0.09*xHO2 + 0.041*xOH + 0.02*xCCHO + 0.075*xRCHO + 0.084*xPROD2 + 0.16*yROOH + 0.02*XC
@ 5.60e-11 ;

R[BP27]= R6OOH -hv-> OH + 0.142*HO2 + 0.782*RO2C + 0.077*RO2XC + 0.077*zRNO3 +
0.085*RCHO + 0.142*PRD2 + 0.782*xHO2 + 0.026*xCCHO + 0.058*xRCHO + 0.698*xPROD2 +
0.858*yR6OOH + 0.017*XC    @ j[COOH_to_HO2] ;
R[BP28]= RAOOH + OH ----> 0.139*OH + 0.148*HO2 + 0.589*RO2C + 0.124*RO2XC + 0.124*zRNO3 +
0.074*PRD2 + 0.147*MGLY + 0.139*IPRD + 0.565*xHO2 + 0.024*xOH + 0.448*xRCHO + 0.026*xGLY +
0.03*xMEK + 0.252*xMGLY + 0.073*xAFG1 + 0.073*xAFG2 + 0.713*yR6OOH + 2.674*XC    @ 1.41e-10 ;

R[BP29]= RAOOH -hv-> OH + HO2 + 0.5*GLY + 0.5*MGLY + 0.5*AFG1 + 0.5*AFG2 + 0.5*XC    @
j[COOH_to_HO2] ;
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NAMES
 PhotoRateIDs += {GLY_to_HO2, GLY_to_CO};
R[BP30]= GLY -hv-> 2*CO + 2*HO2    @ j[GLY_to_HO2] ;

R[BP31]= GLY -hv-> HCHO + CO    @ j[GLY_to_CO] ;
R[BP32]= GLY + OH ----> 0.63*HO2 + 1.26*CO + 0.37*RCO3 + 0.0*XC    @ 1.10e-11 ;
R[BP33]= GLY + NO3 ----> HNO3 + 0.63*HO2 + 1.26*CO + 0.37*RCO3 + 0.0*XC    @ 2.80e-12*EXP(-
2376.0/TK) ;
NAMES
 PhotoRateIDs += {MGLY_to_HO2};
R[BP34]= MGLY -hv-> HO2 + CO + MECO3    @ j[MGLY_to_HO2] ;
R[BP35]= MGLY + OH ----> CO + MECO3    @ 1.50e-11 ;
R[BP36]= MGLY + NO3 ----> HNO3 + CO + MECO3    @ 1.40e-12*EXP(-1895.0/TK) ;
NAMES
 PhotoRateIDs += {CCOCOC_to_RO2};
R[BP37]= BACL -hv-> 2*MECO3    @ j[CCOCOC_to_RO2] ;
R[BP38]= CRES + OH ----> 0.2*BZO + 0.8*RO2C + 0.8*xHO2 + 0.8*yR6OOH + 0.25*xMGLY + 5.05*XC
@ 1.70e-12*EXP(950.0/TK) ;
R[BP39]= CRES + NO3 ----> HNO3 + BZO + XC    @ 1.40e-11 ;
R[BP40]= NPHE + OH ----> BZO + XN    @ 3.50e-12 ;

R[BP41]= NPHE -hv-> HONO + 6*XC    @1.50e-3 *  j[NO2_to_O3P] ;

R[BP42]= NPHE -hv-> 6*XC + XN    @1.50e-2 *  j[NO2_to_O3P] ;
R[BP43]= BALD + OH ----> BZCO3    @ 1.20e-11 ;
NAMES
 PhotoRateIDs += {BzCO_to_NR};
R[BP44]= BALD -hv-> 7*XC    @6.00e-2 *  j[BzCO_to_NR] ;
R[BP45]= BALD + NO3 ----> HNO3 + BZCO3    @ 1.34e-12*EXP(-1860.0/TK) ;
R[BP46]= AFG1 + OH ----> 0.217*MACO3 + 0.723*RO2C + 0.06*RO2XC + 0.06*zRNO3 + 0.521*xHO2 +
0.201*xMECO3 + 0.334*xCO + 0.407*xRCHO + 0.129*xMEK + 0.107*xGLY + 0.267*xMGLY +
0.783*yR6OOH + 0.284*XC    @ 7.40e-11 ;
R[BP47]= AFG1 + O3 ----> 0.826*OH + 0.522*HO2 + 0.652*RO2C + 0.522*CO + 0.174*CO2 +
0.432*GLY + 0.568*MGLY + 0.652*xRCO3 + 0.652*xHCHO + 0.652*yR6OOH + 0.0*XC    @ 9.66e-18 ;
NAMES
 PhotoRateIDs += {AFG1_to_RO2};
R[BP48]= AFG1 -hv-> 1.023*HO2 + 0.173*MEO2 + 0.305*MECO3 + 0.5*MACO3 + 0.695*CO +
0.195*GLY + 0.305*MGLY + 0.217*XC    @ j[AFG1_to_RO2] ;
R[BP49]= AFG2 + OH ----> 0.217*MACO3 + 0.723*RO2C + 0.06*RO2XC + 0.06*zRNO3 + 0.521*xHO2 +
0.201*xMECO3 + 0.334*xCO + 0.407*xRCHO + 0.129*xMEK + 0.107*xGLY + 0.267*xMGLY +
0.783*yR6OOH + 0.284*XC    @ 7.40e-11 ;
R[BP50]= AFG2 + O3 ----> 0.826*OH + 0.522*HO2 + 0.652*RO2C + 0.522*CO + 0.174*CO2 +
0.432*GLY + 0.568*MGLY + 0.652*xRCO3 + 0.652*xHCHO + 0.652*yR6OOH + 0.0*XC    @ 9.66e-18 ;

R[BP51]= AFG2 -hv-> PRD2 + 0.0*XC    @ j[AFG1_to_RO2] ;
R[BP52]= AFG3 + OH ----> 0.206*MACO3 + 0.733*RO2C + 0.117*RO2XC + 0.117*zRNO3 +
0.561*xHO2 + 0.117*xMECO3 + 0.114*xCO + 0.274*xGLY + 0.153*xMGLY + 0.019*xBACL +
0.195*xAFG1 + 0.195*xAFG2 + 0.231*xIPRD + 0.794*yR6OOH + 0.938*XC    @ 9.35e-11 ;
R[BP53a]= AFG3 + O3 ----> 0.471*OH + 0.554*HO2 + 0.013*MECO3 + 0.258*RO2C + 0.007*RO2XC +
                  0.007*zRNO3 + 0.58*CO + 0.19*CO2 + 0.366*GLY + 0.184*MGLY +
                  0.35*(AFG1 + AFG2) + 0.139*AFG3 + 0.003*MACR + 0.004*MVK @ 1.43e-17 ;

R[BP53b]= AFG3 + O3 ----> 0.003*IPRD + 0.095*xHO2 + 0.163*(xRCO3 + xHCHO) + 0.095*xMGLY
                  + 0.264*yR6OOH + 0.0*XC    @ 1.43e-17 ;
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R[BP55]= MACR + O3 ----> 0.208*OH + 0.108*HO2 + 0.1*RO2C + 0.45*CO + 0.117*CO2 + 0.1*HCHO + 0.9*MGLY + 0.333*HCOOH + 0.1*xRCO3 + 0.1*xHCHO + 0.1*yROOH + 0.0*XC @ 1.40e-15*EXP(-2100.0/TK) ;
R[BP56]= MACR + NO3 ----> 0.5*MACO3 + 0.5*RO2C + 0.5*HNO3 + 0.5*xHO2 + 0.5*xCO + 0.5*yROOH + 1.5*XC + 0.5*XN @ 1.50e-12*EXP(-1815.0/TK) ;
R[BP57]= MACR + O3P ----> RCHO + XC @ 6.34e-12 ;
NAMES
PhotoRateIDs += {MACR_to_RO2};
R[BP58]= MACR -hv-> 0.33*OH + 0.67*HO2 + 0.34*MECO3 + 0.33*MACO3 + 0.33*RO2C + 0.67*CO + 0.34*HCHO + 0.33*xMECO3 + 0.33*xHCHO + 0.33*yROOH @ j[MACR_to_RO2] ;
R[BP60]= MVK + O3 ----> 0.164*OH + 0.064*HO2 + 0.05*RO2C + 0.05*xHO2 + 0.475*CO + 0.124*CO2 + 0.05*HCHO + 0.95*MGLY + 0.351*HCOOH + 0.05*xRCO3 + 0.05*xHCHO + 0.05*yROOH + 0.0*XC @ 8.50e-16*EXP(-1520.0/TK) ;
R[BP62]= MVK + O3P ----> 0.45*RCHO + 0.55*MEK + 0.45*XC @ 4.32e-12 ;
NAMES
PhotoRateIDs += {MVK_to_RO2};
R[BP63]= MVK -hv-> 0.4*MEO2 + 0.6*CO + 0.6*PRD2 + 0.4*MACO3 + 0.0*XC @ j[MVK_to_RO2] ;
R[BP64]= IPRD + OH ----> 0.289*MACO3 + 0.67*RO2C + 0.67*xHO2 + 0.041*RO2XC + 0.041*zRNO3 + 0.336*xCO + 0.055*xHCHO + 0.129*xHOCCHO + 0.013*xRCHO + 0.15*xMEK + 0.332*xPROD2 + 0.15*xGLY + 0.174*xMGLY + 0.0*XC + 0.711*yR6OOH @ 6.19e-11 ;
R[BP65]= IPRD + O3 ----> 0.285*OH + 0.4*HO2 + 0.048*RO2C + 0.048*xRCO3 + 0.498*CO + 0.14*CO2 + 0.124*HCHO + 0.21*MEK + 0.023*GLY + 0.742*MGLY + 0.1*HCOOH + 0.372*RCOOH + 0.047*xHOCCHO + 0.001*xHCHO + 0.048*yR6OOH + 0.0*XC @ 4.18e-18 ;
R[BP66]= IPRD + NO3 ----> 0.15*MACO3 + 0.15*HNO3 + 0.799*RO2C + 0.799*xHO2 + 0.051*RO2XC + 0.051*zRNO3 + 0.572*xCO + 0.227*xHCHO + 0.218*xRCHO + 0.008*xMGLY + 0.572*xRNO3 + 0.85*yR6OOH + 0.278*XN + 0.0*XC @ 1.00e-13 ;
R[BP67]= IPRD -hv-> 1.233*HO2 + 0.467*MECO3 + 0.3*RCO3 + 1.233*CO + 0.3*HCHO + 0.467*HOCCHO + 0.233*MEK + 0.0*XC @ j[MACR_to_RO2] ;
R[BP68]= PRD2 + OH ----> 0.472*HO2 + 0.379*xHO2 + 0.029*xMECO3 + 0.049*xRCO3 + 0.473*RO2C + 0.071*RO2XC + 0.071*zRNO3 + 0.002*HCHO + 0.211*xHCHO + 0.001*CCHO + 0.083*xCCHO + 0.143*RCHO + 0.402*xRCHO + 0.115*xMEK + 0.329*PRD2 + 0.007*xPROD2 + 0.528*yR6OOH + 0.877*XC @ 1.55e-11 ;

R[BP69]= PRD2 -hv-> 0.913*xHO2 + 0.4*MECO3 + 0.6*RCO3 + 1.59*RO2C + 0.087*RO2XC + 0.087*zRNO3 + 0.303*xHCHO + 0.163*xCCHO + 0.78*xRCHO + yR6OOH + 0.0*XC @4.86e-3 * j[MVK_to_RO2] ;
R[BP70a]= RNO3 + OH ----> 0.189*HO2 + 0.305*xHO2 + 0.019*NO2 + 0.313*xNO2 + 0.976*RO2C +
0.175*(RO2XC + zRNO3) + 0.011*xHCHO + 0.429*xCCHO +
0.001*RCHO + 0.036*xRCHO + 0.004*xACET + 0.01*MEK + 0.17*xMEK @ 7.20e-12 ;

R[BP70b]= RNO3 + OH ----> 0.008*PRD2 + 0.031*xPROD2 + 0.189*RNO3 + 0.305*xRNO3 +
0.157*yROOH + 0.636*yR6OOH + 0.174*XN + 0.04*XC @ 7.20e-12 ;
NAMES
PhotoRateIDs += {IC3ONO2_to_NO2};
R[BP71]= RNO3 -hv-> 0.344*HO2 + 0.554*xHO2 + NO2 + 0.721*RO2C + 0.102*RO2XC + 0.102*zRNO3 + 0.074*HCHO + 0.061*xHCHO + 0.214*CCHO + 0.23*xCCHO + 0.074*RCHO + 0.063*xRCHO + 0.008*xACETONE + 0.124*MEK + 0.083*xMEK + 0.19*PRD2 + 0.261*xPROD2 + 0.066*yROOH + 0.591*yR6OOH + 0.396*XC @ j[IC3ONO2_to_NO2] ;
R[BP73]= HOCCHO -hv-> CO + 2*HO2 + HCHO @ j[GLY_to_HO2] ;
//R[BP73b]= HOCCHO -hv-> CO + HCHO @ j[GLY_to_CO] ;
R[BP74]= HOCCHO + NO3 ----> HNO3 + MECO3 @ k[BP10] *1.0;
R[BP75]= ACROLEIN + OH ----> 0.25*xHO2 + 0.75*MACO3 + 0.25*RO2C + 0.167*xCO + 0.083*xHCHO + 0.167*xCCHO + 0.083*xGLY + 0.25*yROOH + 0.0*XC @ 1.99e-11 ;
R[BP76]= ACROLEIN + O3 ----> 0.83*HO2 + 0.33*OH + 1.005*CO + 0.31*CO2 + 0.5*HCHO + 0.185*HCOOH + 0.5*GLY @ 1.40e-15*EXP(-2528.0/TK) ;

R[BP77]= ACROLEIN + NO3 ----> 0.031*xHO2 + 0.967*MACO3 + 0.031*RO2C + 0.002*RO2XC + 0.002*zRNO3 + 0.967*HNO3 + 0.031*xCO + 0.031*xRNO3 + 0.033*yROOH + 0.002*XN + 0.0*XC @ 1.18e-15 ;
R[BP78]= ACROLEIN + O3P ----> RCHO @ 2.37e-12 ;
R[BP79]= ACROLEIN -hv-> 1.066*HO2 + 0.178*OH + 0.234*MEO2 + 0.33*MACO3 + 1.188*CO + 0.102*CO2 + 0.34*HCHO + 0.05*CCOOH + 0.0*XC @ j[MACR_to_RO2] ;
R[BP80]= CCOOOH + OH ----> 0.98*MECO3 + 0.02*RO2C + 0.02*CO2 + 0.02*xOH + 0.02*xHCHO + 0.02*yROOH @ 5.28e-12 ;

R[BP81]= CCOOOH -hv-> MEO2 + CO2 + OH @ j[COOH_to_HO2] ;
R[BP82]= RCOOOH + OH ----> 0.806*RCO3 + 0.194*RO2C + 0.194*yROOH + 0.11*CO2 + 0.11*xOH + 0.11*xCCHO + 0.084*xHO2 + 0.084*xRCHO @ 6.42e-12 ;

R[BP83]= RCOOOH -hv-> xHO2 + xCCHO + yROOH + CO2 + OH @ j[COOH_to_HO2] ;
R[P001]= xHCHO + NO ----> NO + HCHO @ k[BR07] *1.0;
R[P002]= xHCHO + HO2 ----> HO2 + XC @ k[BR08] *1.0;
R[P003]= xHCHO + NO3 ----> NO3 + HCHO @ k[BR09] *1.0;
R[P004]= xHCHO + MEO2 ----> MEO2 + 0.5*HCHO + 0.5*XC @ k[BR10] *1.0;
R[P005]= xHCHO + RO2C ----> RO2C + 0.5*HCHO + 0.5*XC @ k[BR11] *1.0;
R[P006]= xHCHO + RO2XC ----> RO2XC + 0.5*HCHO + 0.5*XC @ k[BR11] *1.0;
R[P007]= xHCHO + MECO3 ----> MECO3 + HCHO @ k[BR25] *1.0;
R[P008]= xHCHO + RCO3 ----> RCO3 + HCHO @ k[BR25] *1.0;
R[P009]= xHCHO + BZCO3 ----> BZCO3 + HCHO @ k[BR25] *1.0;
R[P010]= xHCHO + MACO3 ----> MACO3 + HCHO @ k[BR25] *1.0;
R[P011]= xCCHO + NO ----> NO + CCHO @ k[BR07] *1.0;
R[P012]= xCCHO + HO2 ----> HO2 + 2*XC @ k[BR08] *1.0;
R[P013]= xCCHO + NO3 ----> NO3 + CCHO @ k[BR09] *1.0;
R[P014]= xCCHO + MEO2 ----> MEO2 + 0.5*CCHO + XC @ k[BR10] *1.0;
R[P015]= xCCHO + RO2C ----> RO2C + 0.5*CCHO + XC @ k[BR11] *1.0;
R[P016]= xCCHO + RO2XC ----> RO2XC + 0.5*CCHO + XC @ k[BR11] *1.0;
R[P017]= xCCHO + MECO3 ----> MECO3 + CCHO @ k[BR25] *1.0;
R[P018]= xCCHO + RCO3 ----> RCO3 + CCHO @ k[BR25] *1.0;
R[P019]= xCCHO + BZCO3 ----> BZCO3 + CCHO @ k[BR25] *1.0;
R[P020]= xCCHO + MACO3 ----> MACO3 + CCHO @ k[BR25] *1.0;
R[P021]= xRCHO + NO ----> NO + RCHO @ k[BR07] *1.0;
R[P022]= xRCHO + HO2 ----> HO2 + 3*XC @ k[BR08] *1.0;
R[P023]= xRCHO + NO3 ----> NO3 + RCHO @ k[BR09] *1.0;
R[P024]= xRCHO + MEO2 ----> MEO2 + 0.5*RCHO + 1.5*XC @ k[BR10] *1.0;
R[P025]= xRCHO + RO2C ----> RO2C + 0.5*RCHO + 1.5*XC @ k[BR11] *1.0;
R[P026]= xRCHO + RO2XC ----> RO2XC + 0.5*RCHO + 1.5*XC @ k[BR11] *1.0;
R[P027]= xRCHO + MECO3 ----> MECO3 + RCHO @ k[BR25] *1.0;
R[P028]= xRCHO + RCO3 ----> RCO3 + RCHO @ k[BR25] *1.0;
R[P029]= xRCHO + BZCO3 ----> BZCO3 + RCHO @ k[BR25] *1.0;
R[P030]= xRCHO + MACO3 ----> MACO3 + RCHO @ k[BR25] *1.0;
R[P031]= xACETONE + NO ----> NO + ACETONE @ k[BR07] *1.0;
R[P032]= xACETONE + HO2 ----> HO2 + 3*XC @ k[BR08] *1.0;
R[P033]= xACETONE + NO3 ----> NO3 + ACETONE @ k[BR09] *1.0;
R[P034]= xACETONE + MEO2 ----> MEO2 + 0.5*ACETONE + 1.5*XC @ k[BR10] *1.0;
R[P035]= xACETONE + RO2C ----> RO2C + 0.5*ACETONE + 1.5*XC @ k[BR11] *1.0;
R[P036]= xACETONE + RO2XC ----> RO2XC + 0.5*ACETONE + 1.5*XC @ k[BR11] *1.0;
R[P037]= xACETONE + MECO3 ----> MECO3 + ACETONE @ k[BR25] *1.0;
R[P038]= xACETONE + RCO3 ----> RCO3 + ACETONE @ k[BR25] *1.0;
R[P039]= xACETONE + BZCO3 ----> BZCO3 + ACETONE @ k[BR25] *1.0;
R[P040]= xACETONE + MACO3 ----> MACO3 + ACETONE @ k[BR25] *1.0;
R[P041]= xMEK + NO ----> NO + MEK @ k[BR07] *1.0;
R[P042]= xMEK + HO2 ----> HO2 + 4*XC @ k[BR08] *1.0;

R[P043]= xMEK + NO3 ----> NO3 + MEK   @ k[BR09] *1.0;
R[P044]= xMEK + MEO2 ----> MEO2 + 0.5*MEK + 2*XC   @ k[BR10] *1.0;
R[P045]= xMEK + RO2C ----> RO2C + 0.5*MEK + 2*XC   @ k[BR11] *1.0;
R[P046]= xMEK + RO2XC ----> RO2XC + 0.5*MEK + 2*XC   @ k[BR11] *1.0;
R[P047]= xMEK + MECO3 ----> MECO3 + MEK   @ k[BR25] *1.0;
R[P048]= xMEK + RCO3 ----> RCO3 + MEK   @ k[BR25] *1.0;
R[P049]= xMEK + BZCO3 ----> BZCO3 + MEK   @ k[BR25] *1.0;
R[P050]= xMEK + MACO3 ----> MACO3 + MEK   @ k[BR25] *1.0;
R[P051]= xPROD2 + NO ----> NO + PRD2   @ k[BR07] *1.0;
R[P052]= xPROD2 + HO2 ----> HO2 + 6*XC   @ k[BR08] *1.0;
R[P053]= xPROD2 + NO3 ----> NO3 + PRD2   @ k[BR09] *1.0;
R[P054]= xPROD2 + MEO2 ----> MEO2 + 0.5*PRD2 + 3*XC   @ k[BR10] *1.0;
R[P055]= xPROD2 + RO2C ----> RO2C + 0.5*PRD2 + 3*XC   @ k[BR11] *1.0;
R[P056]= xPROD2 + RO2XC ----> RO2XC + 0.5*PRD2 + 3*XC   @ k[BR11] *1.0;
R[P057]= xPROD2 + MECO3 ----> MECO3 + PRD2   @ k[BR25] *1.0;
R[P058]= xPROD2 + RCO3 ----> RCO3 + PRD2   @ k[BR25] *1.0;
R[P059]= xPROD2 + BZCO3 ----> BZCO3 + PRD2   @ k[BR25] *1.0;
R[P060]= xPROD2 + MACO3 ----> MACO3 + PRD2   @ k[BR25] *1.0;
R[P061]= xGLY + NO ----> NO + GLY   @ k[BR07] *1.0;
R[P062]= xGLY + HO2 ----> HO2 + 2*XC   @ k[BR08] *1.0;
R[P063]= xGLY + NO3 ----> NO3 + GLY   @ k[BR09] *1.0;
R[P064]= xGLY + MEO2 ----> MEO2 + 0.5*GLY + XC   @ k[BR10] *1.0;
R[P065]= xGLY + RO2C ----> RO2C + 0.5*GLY + XC   @ k[BR11] *1.0;
R[P066]= xGLY + RO2XC ----> RO2XC + 0.5*GLY + XC   @ k[BR11] *1.0;
R[P067]= xGLY + MECO3 ----> MECO3 + GLY   @ k[BR25] *1.0;
R[P068]= xGLY + RCO3 ----> RCO3 + GLY   @ k[BR25] *1.0;
R[P069]= xGLY + BZCO3 ----> BZCO3 + GLY   @ k[BR25] *1.0;
R[P070]= xGLY + MACO3 ----> MACO3 + GLY   @ k[BR25] *1.0;
R[P071]= xMGLY + NO ----> NO + MGLY   @ k[BR07] *1.0;
R[P072]= xMGLY + HO2 ----> HO2 + 3*XC   @ k[BR08] *1.0;
R[P073]= xMGLY + NO3 ----> NO3 + MGLY   @ k[BR09] *1.0;
R[P074]= xMGLY + MEO2 ----> MEO2 + 0.5*MGLY + 1.5*XC   @ k[BR10] *1.0;
R[P075]= xMGLY + RO2C ----> RO2C + 0.5*MGLY + 1.5*XC   @ k[BR11] *1.0;
R[P076]= xMGLY + RO2XC ----> RO2XC + 0.5*MGLY + 1.5*XC   @ k[BR11] *1.0;
R[P077]= xMGLY + MECO3 ----> MECO3 + MGLY   @ k[BR25] *1.0;
R[P078]= xMGLY + RCO3 ----> RCO3 + MGLY   @ k[BR25] *1.0;
R[P079]= xMGLY + BZCO3 ----> BZCO3 + MGLY   @ k[BR25] *1.0;
R[P080]= xMGLY + MACO3 ----> MACO3 + MGLY   @ k[BR25] *1.0;
R[P081]= xBACL + NO ----> NO + BACL   @ k[BR07] *1.0;
R[P082]= xBACL + HO2 ----> HO2 + 4*XC   @ k[BR08] *1.0;
R[P083]= xBACL + NO3 ----> NO3 + BACL   @ k[BR09] *1.0;
R[P084]= xBACL + MEO2 ----> MEO2 + 0.5*BACL + 2*XC   @ k[BR10] *1.0;
R[P085]= xBACL + RO2C ----> RO2C + 0.5*BACL + 2*XC   @ k[BR11] *1.0;
R[P086]= xBACL + RO2XC ----> RO2XC + 0.5*BACL + 2*XC   @ k[BR11] *1.0;
R[P087]= xBACL + MECO3 ----> MECO3 + BACL   @ k[BR25] *1.0;
R[P088]= xBACL + RCO3 ----> RCO3 + BACL   @ k[BR25] *1.0;
R[P089]= xBACL + BZCO3 ----> BZCO3 + BACL   @ k[BR25] *1.0;
R[P090]= xBACL + MACO3 ----> MACO3 + BACL   @ k[BR25] *1.0;
R[P091]= xBALD + NO ----> NO + BALD   @ k[BR07] *1.0;
R[P092]= xBALD + HO2 ----> HO2 + 7*XC   @ k[BR08] *1.0;
R[P093]= xBALD + NO3 ----> NO3 + BALD   @ k[BR09] *1.0;
R[P094]= xBALD + MEO2 ----> MEO2 + 0.5*BALD + 3.5*XC   @ k[BR10] *1.0;
R[P095]= xBALD + RO2C ----> RO2C + 0.5*BALD + 3.5*XC   @ k[BR11] *1.0;
R[P096]= xBALD + RO2XC ----> RO2XC + 0.5*BALD + 3.5*XC   @ k[BR11] *1.0;
R[P097]= xBALD + MECO3 ----> MECO3 + BALD   @ k[BR25] *1.0;
R[P098]= xBALD + RCO3 ----> RCO3 + BALD   @ k[BR25] *1.0;

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R[P099]= xBALD + BZCO3 ----> BZCO3 + BALD    @ k[BR25] *1.0;
R[P100]= xBALD + MACO3 ----> MACO3 + BALD    @ k[BR25] *1.0;
R[P101]= xAFG1 + NO ----> NO + AFG1    @ k[BR07] *1.0;
R[P102]= xAFG1 + HO2 ----> HO2 + 5*XC    @ k[BR08] *1.0;
R[P103]= xAFG1 + NO3 ----> NO3 + AFG1    @ k[BR09] *1.0;
R[P104]= xAFG1 + MEO2 ----> MEO2 + 0.5*AFG1 + 2.5*XC    @ k[BR10] *1.0;
R[P105]= xAFG1 + RO2C ----> RO2C + 0.5*AFG1 + 2.5*XC    @ k[BR11] *1.0;
R[P106]= xAFG1 + RO2XC ----> RO2XC + 0.5*AFG1 + 2.5*XC    @ k[BR11] *1.0;
R[P107]= xAFG1 + MECO3 ----> MECO3 + AFG1    @ k[BR25] *1.0;
R[P108]= xAFG1 + RCO3 ----> RCO3 + AFG1    @ k[BR25] *1.0;
R[P109]= xAFG1 + BZCO3 ----> BZCO3 + AFG1    @ k[BR25] *1.0;
R[P110]= xAFG1 + MACO3 ----> MACO3 + AFG1    @ k[BR25] *1.0;
R[P111]= xAFG2 + NO ----> NO + AFG2    @ k[BR07] *1.0;
R[P112]= xAFG2 + HO2 ----> HO2 + 5*XC    @ k[BR08] *1.0;
R[P113]= xAFG2 + NO3 ----> NO3 + AFG2    @ k[BR09] *1.0;
R[P114]= xAFG2 + MEO2 ----> MEO2 + 0.5*AFG2 + 2.5*XC    @ k[BR10] *1.0;
R[P115]= xAFG2 + RO2C ----> RO2C + 0.5*AFG2 + 2.5*XC    @ k[BR11] *1.0;
R[P116]= xAFG2 + RO2XC ----> RO2XC + 0.5*AFG2 + 2.5*XC    @ k[BR11] *1.0;
R[P117]= xAFG2 + MECO3 ----> MECO3 + AFG2    @ k[BR25] *1.0;
R[P118]= xAFG2 + RCO3 ----> RCO3 + AFG2    @ k[BR25] *1.0;
R[P119]= xAFG2 + BZCO3 ----> BZCO3 + AFG2    @ k[BR25] *1.0;
R[P120]= xAFG2 + MACO3 ----> MACO3 + AFG2    @ k[BR25] *1.0;
R[P121]= xAFG3 + NO ----> NO + AFG3    @ k[BR07] *1.0;
R[P122]= xAFG3 + HO2 ----> HO2 + 7*XC    @ k[BR08] *1.0;
R[P123]= xAFG3 + NO3 ----> NO3 + AFG3    @ k[BR09] *1.0;
R[P124]= xAFG3 + MEO2 ----> MEO2 + 0.5*AFG3 + 3.5*XC    @ k[BR10] *1.0;
R[P125]= xAFG3 + RO2C ----> RO2C + 0.5*AFG3 + 3.5*XC    @ k[BR11] *1.0;
R[P126]= xAFG3 + RO2XC ----> RO2XC + 0.5*AFG3 + 3.5*XC    @ k[BR11] *1.0;
R[P127]= xAFG3 + MECO3 ----> MECO3 + AFG3    @ k[BR25] *1.0;
R[P128]= xAFG3 + RCO3 ----> RCO3 + AFG3    @ k[BR25] *1.0;
R[P129]= xAFG3 + BZCO3 ----> BZCO3 + AFG3    @ k[BR25] *1.0;
R[P130]= xAFG3 + MACO3 ----> MACO3 + AFG3    @ k[BR25] *1.0;
R[P131]= xMACR + NO ----> NO + MACR    @ k[BR07] *1.0;
R[P132]= xMACR + HO2 ----> HO2 + 4*XC    @ k[BR08] *1.0;
R[P133]= xMACR + NO3 ----> NO3 + MACR    @ k[BR09] *1.0;
R[P134]= xMACR + MEO2 ----> MEO2 + 0.5*MACR + 2*XC    @ k[BR10] *1.0;
R[P135]= xMACR + RO2C ----> RO2C + 0.5*MACR + 2*XC    @ k[BR11] *1.0;
R[P136]= xMACR + RO2XC ----> RO2XC + 0.5*MACR + 2*XC    @ k[BR11] *1.0;
R[P137]= xMACR + MECO3 ----> MECO3 + MACR    @ k[BR25] *1.0;
R[P138]= xMACR + RCO3 ----> RCO3 + MACR    @ k[BR25] *1.0;
R[P139]= xMACR + BZCO3 ----> BZCO3 + MACR    @ k[BR25] *1.0;
R[P140]= xMACR + MACO3 ----> MACO3 + MACR    @ k[BR25] *1.0;
R[P141]= xMVK + NO ----> NO + MVK    @ k[BR07] *1.0;
R[P142]= xMVK + HO2 ----> HO2 + 4*XC    @ k[BR08] *1.0;
R[P143]= xMVK + NO3 ----> NO3 + MVK    @ k[BR09] *1.0;
R[P144]= xMVK + MEO2 ----> MEO2 + 0.5*MVK + 2*XC    @ k[BR10] *1.0;
R[P145]= xMVK + RO2C ----> RO2C + 0.5*MVK + 2*XC    @ k[BR11] *1.0;
R[P146]= xMVK + RO2XC ----> RO2XC + 0.5*MVK + 2*XC    @ k[BR11] *1.0;
R[P147]= xMVK + MECO3 ----> MECO3 + MVK    @ k[BR25] *1.0;
R[P148]= xMVK + RCO3 ----> RCO3 + MVK    @ k[BR25] *1.0;
R[P149]= xMVK + BZCO3 ----> BZCO3 + MVK    @ k[BR25] *1.0;
R[P150]= xMVK + MACO3 ----> MACO3 + MVK    @ k[BR25] *1.0;
R[P151]= xIPRD + NO ----> NO + IPRD    @ k[BR07] *1.0;
R[P152]= xIPRD + HO2 ----> HO2 + 5*XC    @ k[BR08] *1.0;
R[P153]= xIPRD + NO3 ----> NO3 + IPRD    @ k[BR09] *1.0;
R[P154]= xIPRD + MEO2 ----> MEO2 + 0.5*IPRD + 2.5*XC    @ k[BR10] *1.0;
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R[P155]= xIPRD + RO2C ----> RO2C + 0.5*IPRD + 2.5*XC    @ k[BR11] *1.0;
R[P156]= xIPRD + RO2XC ----> RO2XC + 0.5*IPRD + 2.5*XC    @ k[BR11] *1.0;
R[P157]= xIPRD + MECO3 ----> MECO3 + IPRD    @ k[BR25] *1.0;
R[P158]= xIPRD + RCO3 ----> RCO3 + IPRD    @ k[BR25] *1.0;
R[P159]= xIPRD + BZCO3 ----> BZCO3 + IPRD    @ k[BR25] *1.0;
R[P160]= xIPRD + MACO3 ----> MACO3 + IPRD    @ k[BR25] *1.0;
R[P161]= xRNO3 + NO ----> NO + RNO3    @ k[BR07] *1.0;
R[P162]= xRNO3 + HO2 ----> HO2 + 6*XC + XN    @ k[BR08] *1.0;
R[P163]= xRNO3 + NO3 ----> NO3 + RNO3    @ k[BR09] *1.0;
R[P164]= xRNO3 + MEO2 ----> MEO2 + 0.5*RNO3 + 0.5*XN + 3*XC    @ k[BR10] *1.0;
R[P165]= xRNO3 + RO2C ----> RO2C + 0.5*RNO3 + 0.5*XN + 3*XC    @ k[BR11] *1.0;
R[P166]= xRNO3 + RO2XC ----> RO2XC + 0.5*RNO3 + 0.5*XN + 3*XC    @ k[BR11] *1.0;
R[P167]= xRNO3 + MECO3 ----> MECO3 + RNO3    @ k[BR25] *1.0;
R[P168]= xRNO3 + RCO3 ----> RCO3 + RNO3    @ k[BR25] *1.0;
R[P169]= xRNO3 + BZCO3 ----> BZCO3 + RNO3    @ k[BR25] *1.0;
R[P170]= xRNO3 + MACO3 ----> MACO3 + RNO3    @ k[BR25] *1.0;
R[P171]= yROOH + NO ----> NO    @ k[BR07] *1.0;
R[P172]= yROOH + HO2 ----> HO2 + ROOH + 0.0*XC    @ k[BR08] *1.0;
R[P173]= yROOH + NO3 ----> NO3    @ k[BR09] *1.0;
R[P174]= yROOH + MEO2 ----> MEO2 + 0.5*MEK + 0.0*XC    @ k[BR10] *1.0;
R[P175]= yROOH + RO2C ----> RO2C + 0.5*MEK + 0.0*XC    @ k[BR11] *1.0;
R[P176]= yROOH + RO2XC ----> RO2XC + 0.5*MEK + 0.0*XC    @ k[BR11] *1.0;
R[P177]= yROOH + MECO3 ----> MECO3    @ k[BR25] *1.0;
R[P178]= yROOH + RCO3 ----> RCO3    @ k[BR25] *1.0;
R[P179]= yROOH + BZCO3 ----> BZCO3    @ k[BR25] *1.0;
R[P180]= yROOH + MACO3 ----> MACO3    @ k[BR25] *1.0;
R[P181]= yR6OOH + NO ----> NO    @ k[BR07] *1.0;
R[P182]= yR6OOH + HO2 ----> HO2 + R6OOH + 0.0*XC    @ k[BR08] *1.0;
R[P183]= yR6OOH + NO3 ----> NO3    @ k[BR09] *1.0;
R[P184]= yR6OOH + MEO2 ----> MEO2 + 0.5*PRD2 + 0.0*XC    @ k[BR10] *1.0;
R[P185]= yR6OOH + RO2C ----> RO2C + 0.5*PRD2 + 0.0*XC    @ k[BR11] *1.0;
R[P186]= yR6OOH + RO2XC ----> RO2XC + 0.5*PRD2 + 0.0*XC    @ k[BR11] *1.0;
R[P187]= yR6OOH + MECO3 ----> MECO3    @ k[BR25] *1.0;
R[P188]= yR6OOH + RCO3 ----> RCO3    @ k[BR25] *1.0;
R[P189]= yR6OOH + BZCO3 ----> BZCO3    @ k[BR25] *1.0;
R[P190]= yR6OOH + MACO3 ----> MACO3    @ k[BR25] *1.0;
R[P191]= yRAOOH + NO ----> NO    @ k[BR07] *1.0;
R[P192]= yRAOOH + HO2 ----> HO2 + RAOOH + 0.0*XC    @ k[BR08] *1.0;
R[P193]= yRAOOH + NO3 ----> NO3    @ k[BR09] *1.0;
R[P194]= yRAOOH + MEO2 ----> MEO2 + 0.5*PRD2 + 0.0*XC    @ k[BR10] *1.0;
R[P195]= yRAOOH + RO2C ----> RO2C + 0.5*PRD2 + 0.0*XC    @ k[BR11] *1.0;
R[P196]= yRAOOH + RO2XC ----> RO2XC + 0.5*PRD2 + 0.0*XC    @ k[BR11] *1.0;
R[P197]= yRAOOH + MECO3 ----> MECO3    @ k[BR25] *1.0;
R[P198]= yRAOOH + RCO3 ----> RCO3    @ k[BR25] *1.0;
R[P199]= yRAOOH + BZCO3 ----> BZCO3    @ k[BR25] *1.0;
R[P200]= yRAOOH + MACO3 ----> MACO3    @ k[BR25] *1.0;
R[P201]= zRNO3 + NO ----> NO + RNO3    @ k[BR07] *1.0;
R[P202]= zRNO3 + HO2 ----> HO2 + 6*XC    @ k[BR08] *1.0;
R[P203]= zRNO3 + NO3 ----> NO3 + PRD2 + HO2    @ k[BR09] *1.0;
R[P204]= zRNO3 + MEO2 ----> MEO2 + 0.5*PRD2 + 0.5*HO2 + 3*XC    @ k[BR10] *1.0;
R[P205]= zRNO3 + RO2C ----> RO2C + 0.5*PRD2 + 0.5*HO2 + 3*XC    @ k[BR11] *1.0;
R[P206]= zRNO3 + RO2XC ----> RO2XC + 0.5*PRD2 + 0.5*HO2 + 3*XC    @ k[BR11] *1.0;
R[P207]= zRNO3 + MECO3 ----> MECO3 + PRD2 + HO2    @ k[BR25] *1.0;
R[P208]= zRNO3 + RCO3 ----> RCO3 + PRD2 + HO2    @ k[BR25] *1.0;
R[P209]= zRNO3 + BZCO3 ----> BZCO3 + PRD2 + HO2    @ k[BR25] *1.0;
R[P210]= zRNO3 + MACO3 ----> MACO3 + PRD2 + HO2    @ k[BR25] *1.0;
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R[P211]= xHOCCHO + NO ----> NO + HOCCHO    @ k[BR07] *1.0;
R[P212]= xHOCCHO + HO2 ----> HO2 + 2*XC    @ k[BR08] *1.0;
R[P213]= xHOCCHO + NO3 ----> NO3 + HOCCHO    @ k[BR09] *1.0;
R[P214]= xHOCCHO + MEO2 ----> MEO2 + 0.5*HOCCHO + XC    @ k[BR10] *1.0;
R[P215]= xHOCCHO + RO2C ----> RO2C + 0.5*HOCCHO + XC    @ k[BR11] *1.0;
R[P216]= xHOCCHO + RO2XC ----> RO2XC + 0.5*HOCCHO + XC    @ k[BR11] *1.0;
R[P217]= xHOCCHO + MECO3 ----> MECO3 + HOCCHO    @ k[BR25] *1.0;
R[P218]= xHOCCHO + RCO3 ----> RCO3 + HOCCHO    @ k[BR25] *1.0;
R[P219]= xHOCCHO + BZCO3 ----> BZCO3 + HOCCHO    @ k[BR25] *1.0;
R[P220]= xHOCCHO + MACO3 ----> MACO3 + HOCCHO    @ k[BR25] *1.0;
R[P221]= xACROLEIN + NO ----> NO + ACROLEIN    @ k[BR07] *1.0;
R[P222]= xACROLEIN + HO2 ----> HO2 + 3*XC    @ k[BR08] *1.0;
R[P223]= xACROLEIN + NO3 ----> NO3 + ACROLEIN    @ k[BR09] *1.0;
R[P224]= xACROLEIN + MEO2 ----> MEO2 + 0.5*ACROLEIN + 1.5*XC    @ k[BR10] *1.0;
R[P225]= xACROLEIN + RO2C ----> RO2C + 0.5*ACROLEIN + 1.5*XC    @ k[BR11] *1.0;
R[P226]= xACROLEIN + RO2XC ----> RO2XC + 0.5*ACROLEIN + 1.5*XC    @ k[BR11] *1.0;
R[P227]= xACROLEIN + MECO3 ----> MECO3 + ACROLEIN    @ k[BR25] *1.0;
R[P228]= xACROLEIN + RCO3 ----> RCO3 + ACROLEIN    @ k[BR25] *1.0;
R[P229]= xACROLEIN + BZCO3 ----> BZCO3 + ACROLEIN    @ k[BR25] *1.0;
R[P230]= xACROLEIN + MACO3 ----> MACO3 + ACROLEIN    @ k[BR25] *1.0;
R[BE01]= CH4 + OH ----> MEO2    @ 1.85e-12*EXP(-1690.0/TK) ;
R[BE02]= ETHE + OH ----> xHO2 + RO2C + 1.61*xHCHO + 0.195*xHOCCHO + yROOH    @
TROE( 1.00e-28*(T_300)^-4.50,  8.80e-12*(T_300)^-0.85, b[M],0.60) ;
R[BE03]= ETHE + O3 ----> 0.16*HO2 + 0.16*OH + 0.51*CO + 0.12*CO2 + HCHO + 0.37*HCOOH    @
9.14e-15*EXP(-2580.0/TK) ;
R[BE04]= ETHE + NO3 ----> xHO2 + RO2C + xRCHO + yROOH + XN + 0.0*XC    @ 3.30e-
12*(T_300)^2.00*EXP(-2880.0/TK) ;
R[BE05]= ETHE + O3P ----> 0.8*HO2 + 0.29*xHO2 + 0.51*MEO2 + 0.29*RO2C + 0.51*CO + 0.278*xCO
+ 0.278*xHCHO + 0.1*CCHO + 0.012*xGLY + 0.29*yROOH + 0.2*XC    @ 1.07e-11*EXP(-800.0/TK) ;

R[BT01]= PROPENE + OH ----> 0.984*xHO2 + 0.984*RO2C + 0.016*RO2XC + 0.016*zRNO3 +
0.984*xHCHO + 0.984*xCCHO + yROOH + 0.0*XC    @ 4.85e-12*EXP(504.0/TK) ;
R[BT02]= PROPENE + O3 ----> 0.165*HO2 + 0.35*OH + 0.355*MEO2 + 0.525*CO + 0.215*CO2 +
0.5*HCHO + 0.5*CCHO + 0.185*HCOOH + 0.075*CCOOH + 0.07*XC    @ 5.51e-15*EXP(-1878.0/TK) ;
R[BT03]= PROPENE + NO3 ----> 0.949*xHO2 + 0.949*RO2C + 0.051*RO2XC + 0.051*zRNO3 + yROOH
+ XN + 2.694*XC    @ 4.59e-13*EXP(-1156.0/TK) ;
R[BT04]= PROPENE + O3P ----> 0.45*RCHO + 0.55*MEK + 0.0*XC    @ 1.02e-11*EXP(-280.0/TK) ;
R[BT05]= BUTADIENE13 + OH ----> 0.951*xHO2 + 1.189*RO2C + 0.049*RO2XC + 0.049*zRNO3 +
0.708*xHCHO + 0.48*xACROLEIN + 0.471*xIPRD + yROOH + 0.0*XC    @ 1.48e-11*EXP(448.0/TK) ;
R[BT06]= BUTADIENE13 + O3 ----> 0.08*HO2 + 0.08*OH + 0.255*CO + 0.185*CO2 + 0.5*HCHO +
0.185*HCOOH + 0.5*ACROLEIN + 0.375*MVK + 0.125*PRD2 + 0.0*XC    @ 1.34e-14*EXP(-2283.0/TK) ;
R[BT07]= BUTADIENE13 + NO3 ----> 0.815*xHO2 + 0.12*xNO2 + 1.055*RO2C + 0.065*RO2XC +
0.065*zRNO3 + 0.115*xHCHO + 0.46*xMVK + 0.12*xIPRD + 0.355*xRNO3 + yROOH + 0.525*XN +
0.0*XC    @ 1.00e-13 ;
R[BT08]= BUTADIENE13 + O3P ----> 0.25*HO2 + 0.117*xHO2 + 0.118*xMACO3 + 0.235*RO2C +
0.015*RO2XC + 0.015*zRNO3 + 0.115*xCO + 0.115*xACROLEIN + 0.001*xAFG1 + 0.001*xAFG2 +
0.75*PRD2 + 0.25*yROOH + 0.0*XC    @ 2.26e-11*EXP(-40.0/TK) ;
R[BE07]= ISOP + O3 ----> 0.066*HO2 + 0.266*OH + 0.192*xMACO3 + 0.192*RO2C + 0.008*RO2XC +
0.008*zRNO3 + 0.275*CO + 0.122*CO2 + 0.4*HCHO + 0.192*xHCHO + 0.204*HCOOH + 0.39*MACR +
0.16*MVK + 0.15*IPRD + 0.1*PRD2 + 0.2*yR6OOH + 0.0*XC    @ 7.86e-15*EXP(-1912.0/TK) ;
R[BE09]= ISOP + O3P ----> 0.25*MEO2 + 0.24*xMACO3 + 0.24*RO2C + 0.01*RO2XC + 0.01*zRNO3 +
0.24*xHCHO + 0.75*PRD2 + 0.25*yR6OOH + 0.0*XC    @ 3.50e-11 ;
R[BT09]= APIN + OH ----> 0.799*xHO2 + 0.004*xRCO3 + 1.042*RO2C + 0.197*RO2XC + 0.197*zRNO3
+ 0.002*xCO + 0.022*xHCHO + 0.776*xRCHO + 0.034*xACETONE + 0.02*xMGLY + 0.023*xBACL +
yR6OOH + TRPRXN + 6.2*XC    @ 1.21e-11*EXP(436.0/TK) ;
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R[BT10]= APIN + O3 ----> 0.009*HO2 + 0.102*xHO2 + 0.728*OH + 0.001*xMECO3 + 0.297*xRCO3 + 1.511*RO2C + 0.337*RO2XC + 0.337*zRNO3 + 0.029*CO + 0.051*xCO + 0.017*CO2 + 0.344*xHCHO + 0.24*xRCHO + 0.345*xACETONE + 0.008*MEK + 0.002*xGLY + 0.081*xBACL + 0.255*PRD2 + 0.737*yR6OOH + TRPRXN + 2.999*XC @ 5.00e-16*EXP(-530.0/TK) ;
R[BT11]= APIN + NO3 ----> 0.056*xHO2 + 0.643*xNO2 + 0.007*xRCO3 + 1.05*RO2C + 0.293*RO2XC + 0.293*zRNO3 + 0.005*xCO + 0.007*xHCHO + 0.684*xRCHO + 0.069*xACETONE + 0.002*xMGLY + 0.056*xRNO3 + yR6OOH + 0.301*XN + TRPRXN + 5.608*XC @ 1.19e-12*EXP(490.0/TK) ;
R[BT12]= APIN + O3P ----> PRD2 + TRPRXN + 4*XC @ 3.20e-11 ;
R[BE10]= ACYE + OH ----> 0.3*HO2 + 0.7*OH + 0.3*CO + 0.3*HCOOH + 0.7*GLY @ TROE(5.50e-30*(T_300)^-2.00, 8.30e-13, b[M],0.60) ;
R[BE11]= ACYE + O3 ----> 1.5*HO2 + 0.5*OH + 1.5*CO + 0.5*CO2 @ 1.00e-14*EXP(-4100.0/TK) ;
R[BE12]= BENZENE + OH ----> 0.57*HO2 + 0.29*xHO2 + 0.116*OH + 0.29*RO2C + 0.024*RO2XC + 0.024*zRNO3 + 0.29*xGLY + 0.57*CRES + 0.029*xAFG1 + 0.261*xAFG2 + 0.116*AFG3 + 0.314*yRAOOH + BENZRO2 + 0.0*XC @ 2.33e-12*EXP(-193.0/TK) ;
R[BT13]= TOLUENE + OH ----> 0.181*HO2 + 0.454*xHO2 + 0.312*OH + 0.454*RO2C + 0.054*RO2XC + 0.054*zRNO3 + 0.238*xGLY + 0.151*xMGLY + 0.181*CRES + 0.065*xBALD + 0.195*xAFG1 + 0.195*xAFG2 + 0.312*AFG3 + 0.073*yR6OOH + 0.435*yRAOOH + TOLRO2 + 0.0*XC @ 1.81e-12*EXP(338.0/TK) ;
R[BT14]= MXYL + OH ----> 0.159*HO2 + 0.52*xHO2 + 0.239*OH + 0.52*RO2C + 0.082*RO2XC + 0.082*zRNO3 + 0.1*xGLY + 0.38*xMGLY + 0.159*CRES + 0.041*xBALD + 0.336*xAFG1 + 0.144*xAFG2 + 0.239*AFG3 + 0.047*yR6OOH + 0.555*yRAOOH + XYLRO2 + 0.695*XC @ 2.31e-11 ;
R[BT15]= OXYL + OH ----> 0.161*HO2 + 0.554*xHO2 + 0.198*OH + 0.554*RO2C + 0.087*RO2XC + 0.087*zRNO3 + 0.084*xGLY + 0.238*xMGLY + 0.185*xBACL + 0.161*CRES + 0.047*xBALD + 0.253*xAFG1 + 0.253*xAFG2 + 0.198*AFG3 + 0.055*yR6OOH + 0.586*yRAOOH + XYLRO2 + 0.484*XC @ 1.36e-11 ;
R[BT16]= PXYL + OH ----> 0.159*HO2 + 0.487*xHO2 + 0.278*OH + 0.487*RO2C + 0.076*RO2XC + 0.076*zRNO3 + 0.286*xGLY + 0.112*xMGLY + 0.159*CRES + 0.088*xBALD + 0.045*xAFG1 + 0.067*xAFG2 + 0.278*AFG3 + 0.286*xAFG3 + 0.102*yR6OOH + 0.461*yRAOOH + XYLRO2 + 0.399*XC @ 1.43e-11 ;
R[BT17]= TRIMETH + BENZ124 + OH ----> 0.022*HO2 + 0.627*xHO2 + 0.23*OH + 0.627*RO2C + 0.121*RO2XC + 0.121*zRNO3 + 0.074*xGLY + 0.405*xMGLY + 0.112*xBACL + 0.022*CRES + 0.036*xBALD + 0.088*xAFG1 + 0.352*xAFG2 + 0.23*AFG3 + 0.151*xAFG3 + 0.043*yR6OOH + 0.705*yRAOOH + XYLRO2 + 1.19*XC @ 3.25e-11 ;
R[BT18]= ETOH + OH ----> 0.95*HO2 + 0.05*xHO2 + 0.05*RO2C + 0.081*xHCHO + 0.95*CCHO + 0.01*xHOCCHO + 0.05*yROOH + 0.0*XC @ 5.49e-13*(T_300)^2.00*EXP(530.0/TK) ;
R[BL01]= ALK1 + OH ----> xHO2 + RO2C + xCCHO + yROOH @ 1.34e-12*(T_300)^2.00*EXP(-499.0/TK) ;
R[BL02]= ALK2 + OH ----> 0.965*xHO2 + 0.965*RO2C + 0.035*RO2XC + 0.035*zRNO3 + 0.261*xRCHO + 0.704*xACETONE + yROOH + 0.0*XC @ 1.49e-12*(T_300)^2.00*EXP(-87.0/TK) ;
R[BL03]= ALK3 + OH ----> 0.695*xHO2 + 0.236*xTBUO + 1.253*RO2C + 0.07*RO2XC + 0.07*zRNO3 + 0.026*xHCHO + 0.445*xCCHO + 0.122*xRCHO + 0.024*xACETONE + 0.332*xMEK + 0.983*yROOH + 0.017*yR6OOH + 0.0*XC @ 1.51e-12*EXP(126.0/TK) ;
R[BL04]= ALK4 + OH ----> 0.83*xHO2 + 0.01*xMEO2 + 0.011*xMECO3 + 1.763*RO2C + 0.149*RO2XC + 0.149*zRNO3 + 0.002*xCO + 0.029*xHCHO + 0.438*xCCHO + 0.236*xRCHO + 0.426*xACETONE + 0.106*xMEK + 0.146*xPROD2 + yR6OOH + 0.0*XC @ 3.75e-12*EXP(44.0/TK) ;
R[BL05]= ALK5 + OH ----> 0.647*xHO2 + 1.605*RO2C + 0.353*RO2XC + 0.353*zRNO3 + 0.04*xHCHO + 0.106*xCCHO + 0.209*xRCHO + 0.071*xACETONE + 0.086*xMEK + 0.407*xPROD2 + yR6OOH + ALK5RXN + 2.004*XC @ 2.70e-12*EXP(374.0/TK) ;
R[BL06]= OLE1 + OH ----> 0.871*xHO2 + 0.001*xMEO2 + 1.202*RO2C + 0.128*RO2XC + 0.128*zRNO3 + 0.582*xHCHO + 0.01*xCCHO + 0.007*xHOCCHO + 0.666*xRCHO + 0.007*xACETONE + 0.036*xACROLEIN + 0.001*xMACR + 0.012*xMVK + 0.009*xIPRD + 0.168*xPROD2 + 0.169*yROOH + 0.831*yR6OOH + 0.383*XC @ 6.72e-12*EXP(501.0/TK) ;
R[BL07]= OLE1 + O3 ----> 0.095*HO2 + 0.057*xHO2 + 0.128*OH + 0.09*RO2C + 0.005*RO2XC + 0.005*zRNO3 + 0.303*CO + 0.088*CO2 + 0.5*HCHO + 0.011*xCCHO + 0.5*RCHO + 0.044*xRCHO + 0.003*xACETONE + 0.009*MEK + 0.185*HCOOH + 0.159*RCOOH + 0.268*PRD2 + 0.011*yROOH + 0.052*yR6OOH + 0.11*XC @ 3.19e-15*EXP(-1701.0/TK) ;

R[BL08]= OLE1 + NO3 ----> 0.772*xHO2 + 1.463*RO2C + 0.228*RO2XC + 0.228*zRNO3 + 0.013*xCCHO + 0.003*xRCHO + 0.034*xACETONE + 0.774*xRNO3 + 0.169*yROOH + 0.831*yR6OOH + 0.226*XN + 0.0*XC @ 5.37e-13*EXP(-1047.0/TK) ;
R[BL09]= OLE1 + O3P ----> 0.45*RCHO + 0.39*MEK + 0.16*PRD2 + 1.13*XC @ 1.61e-11*EXP(-326.0/TK) ;
R[BL10]= OLE2 + OH ----> 0.912*xHO2 + 0.953*RO2C + 0.088*RO2XC + 0.088*zRNO3 + 0.179*xHCHO + 0.835*xCCHO + 0.51*xRCHO + 0.144*xACETONE + 0.08*xMEK + 0.002*xMVK + 0.012*xIPRD + 0.023*xPROD2 + 0.319*yROOH + 0.681*yR6OOH + 0.135*XC @ 1.26e-11*EXP(488.0/TK) ;
R[BL11a]= OLE2 + O3 ----> 0.093*HO2 + 0.039*xHO2 + 0.423*OH + 0.29*MEO2 + 0.147*xMECO3 + 0.008*xRCO3 + 0.2*RO2C + 0.003*(RO2XC + zRNO3) + 0.297*CO + 0.162*CO2 + 0.152*HCHO + 0.108*xHCHO + 0.428*CCHO + 0.067*xCCHO @ 8.14e-15*EXP(-1255.0/TK) ;

R[BL11b]= OLE2 + O3 ----> 0.315*RCHO + 0.018*xRCHO + 0.048*ACET + 0.031*MEK + 0.001*xMEK + 0.033*FACD + 0.061*AACD + 0.222*PACD + 0.028*MACR + 0.021*MVK + 0.042*PRD2 + 0.069*yROOH + 0.128*yR6OOH + 0.125*XC @ 8.14e-15*EXP(-1255.0/TK) ;
R[BL12]= OLE2 + NO3 ----> 0.4*xHO2 + 0.426*xNO2 + 0.035*xMEO2 + 1.193*RO2C + 0.14*RO2XC + 0.14*zRNO3 + 0.072*xHCHO + 0.579*xCCHO + 0.163*xRCHO + 0.116*xACETONE + 0.002*xMEK + 0.32*xRNO3 + 0.319*yROOH + 0.681*yR6OOH + 0.254*XN + 0.13*XC @ 2.31e-13*EXP(382.0/TK) ;
R[BL13]= OLE2 + O3P ----> 0.079*RCHO + 0.751*MEK + 0.17*PRD2 + 0.739*XC @ 1.43e-11*EXP(111.0/TK) ;
R[BL14]= ARO1 + OH ----> 0.123*HO2 + 0.566*xHO2 + 0.202*OH + 0.566*RO2C + 0.11*RO2XC + 0.11*zRNO3 + 0.158*xGLY + 0.1*xMGLY + 0.123*CRES + 0.072*xAFG1 + 0.185*xAFG2 + 0.202*AFG3 + 0.309*xPROD2 + 0.369*yR6OOH + TOLRO2 + 0.31*XC @ 7.84e-12 ;
R[BL15]= ARO2 + OH ----> 0.077*HO2 + 0.617*xHO2 + 0.178*OH + 0.617*RO2C + 0.128*RO2XC + 0.128*zRNO3 + 0.088*xGLY + 0.312*xMGLY + 0.134*xBACL + 0.077*CRES + 0.026*xBALD + 0.221*xAFG1 + 0.247*xAFG2 + 0.178*AFG3 + 0.068*xAFG3 + 0.057*xPROD2 + 0.101*yR6OOH + XYLRO2 + 1.459*XC @ 3.09e-11 ;
R[BL16]= TERP + OH ----> 0.734*xHO2 + 0.064*xRCO3 + 1.211*RO2C + 0.201*RO2XC + 0.201*zRNO3 + 0.001*xCO + 0.411*xHCHO + 0.385*xRCHO + 0.037*xACETONE + 0.007*xMEK + 0.003*xMGLY + 0.009*xBACL + 0.003*xMVK + 0.002*xIPRD + 0.409*xPROD2 + yR6OOH + TRPRXN + 4.375*XC @ 2.27e-11*EXP(435.0/TK) ;
R[BL17a]= TERP + O3 ----> 0.052*HO2 + 0.067*xHO2 + 0.585*OH + 0.126*xMECO3 + 0.149*xRCO3 + 0.875*RO2C + 0.203*RO2XC + 0.203*zRNO3 + 0.166*CO + 0.019*xCO + 0.045*CO2 + 0.079*HCHO + 0.15*xHCHO + 0.22*xRCHO + 0.165*xACET @ 9.57e-16*EXP(-785.0/TK) ;

R[BL17b]= TERP + O3 ----> 0.004*MEK + 0.107*FACD + 0.043*PACD + 0.001*xGLY + 0.002*xMGLY + 0.055*xBACL + 0.001*xMACR + 0.001*xIPRD + 0.409*PRD2 + 0.545*yR6OOH + 3.526*XC @ 9.57e-16*EXP(-785.0/TK) ;
R[BL18]= TERP + NO3 ----> 0.227*xHO2 + 0.287*xNO2 + 0.026*xRCO3 + 1.786*RO2C + 0.46*RO2XC + 0.46*zRNO3 + 0.012*xCO + 0.023*xHCHO + 0.002*xHOCCHO + 0.403*xRCHO + 0.239*xACETONE + 0.005*xMACR + 0.001*xMVK + 0.004*xIPRD + 0.228*xRNO3 + yR6OOH + TRPRXN + 0.485*XN + 3.785*XC @ 1.33e-12*EXP(490.0/TK) ;
R[BL19]= TERP + O3P ----> 0.237*RCHO + 0.763*PRD2 + TRPRXN + 4.711*XC @ 4.02e-11 ;
R[BT19]= SESQ + OH ----> 0.734*xHO2 + 0.064*xRCO3 + 1.211*RO2C + 0.201*RO2XC + 0.201*zRNO3 + 0.001*xCO + 0.411*xHCHO + 0.385*xRCHO + 0.037*xACETONE + 0.007*xMEK + 0.003*xMGLY + 0.009*xBACL + 0.003*xMVK + 0.002*xIPRD + 0.409*xPROD2 + yR6OOH + SESQRXN + 9.375*XC @ k[BL16] *1.0;
R[BT20a]= SESQ + O3 ----> 0.078*HO2 + 0.046*xHO2 + 0.499*OH + 0.202*xMECO3 + 0.059*xRCO3 + 0.49*RO2C + 0.121*RO2XC + 0.121*zRNO3 + 0.249*CO + 0.063*CO2 + 0.127*HCHO @ k[BL17a] *1.0;
R[BT20b]= SESQ + O3 ----> 0.033*xHCHO + 0.208*xRCHO + 0.057*xACETONE + 0.002*MEK + 0.172*HCOOH + 0.068*RCOOH + 0.003*xMGLY + 0.039*xBACL + 0.002*xMACR + 0.001*xIPRD + 0.502*PRD2 + 0.428*yR6OOH + SESQRXN + 8.852*XC @ k[BL17a] *1.0;

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R[BT21]= SESQ + NO3 ----> 0.227*xHO2 + 0.287*xNO2 + 0.026*xRCO3 + 1.786*RO2C + 0.46*RO2XC
+ 0.46*zRNO3 + 0.012*xCO + 0.023*xHCHO + 0.002*xCCHO + 0.403*xRCHO + 0.239*xACETONE +
0.005*xMACR + 0.001*xMVK + 0.004*xIPRD + 0.228*xRNO3 + yR6OOH + SESQRXN + 0.485*XN +
8.785*XC    @ k[BL18] *1.0;
R[BT22]= SESQ + O3P ----> 0.237*RCHO + 0.763*PRD2 + SESQRXN + 9.711*XC    @ k[BL19] *1.0;
/*NAMES
 PhotoRateIDs += {CL2};
R[CI01]= CL2 -hv-> 2*CL    @ j[CL2] ;
R[CI02]= CL + NO + M ----> CLNO    @ 7.60e-32*(T_300)^-1.80 ;
NAMES
 PhotoRateIDs += {CLNO-06};
R[CI03]= CLNO -hv-> CL + NO    @ j[CLNO-06] ;
R[CI04]= CL + NO2 ----> CLONO    @ TROE( 1.30e-30*(T_300)^-2.00,  1.00e-10*(T_300)^-1.00,
b[M],0.60) ;
R[CI05]= CL + NO2 ----> CLNO2    @ TROE( 1.80e-31*(T_300)^-2.00,  1.00e-10*(T_300)^-1.00,
b[M],0.60) ;
NAMES
 PhotoRateIDs += {CLONO};
R[CI06]= CLONO -hv-> CL + NO2    @ j[CLONO] ;
NAMES
 PhotoRateIDs += {CLNO2};
R[CI07]= CLNO2 -hv-> CL + NO2    @ j[CLNO2] ;
R[CI08]= CL + HO2 ----> HCL    @ 3.44e-11*(T_300)^-0.56 ;
R[CI09]= CL + HO2 ----> CLO + OH    @ 9.41e-12*(T_300)^2.10 ;
R[CI10]= CL + O3 ----> CLO    @ 2.80e-11*EXP(-250.0/TK) ;
R[CI11]= CL + NO3 ----> CLO + NO2    @ 2.40e-11 ;
R[CI12]= CLO + NO ----> CL + NO2    @ 6.20e-12*EXP(295.0/TK) ;
R[CI13]= CLO + NO2 ----> CLONO2    @ TROE( 1.80e-31*(T_300)^-3.40,  1.50e-11*(T_300)^-1.90,
b[M],0.60) ;
NAMES
 PhotoRateIDs += {CLONO2-1};
R[CI14]= CLONO2 -hv-> CLO + NO2    @ j[CLONO2-1] ;
NAMES
 PhotoRateIDs += {CLONO2-2};
R[CI15]= CLONO2 -hv-> CL + NO3    @ j[CLONO2-2] ;
R[CI16]= CLONO2 ----> CLO + NO2    @ TROE( 4.48e-05*(T_300)^-1.00*EXP(-12530.0/TK),
3.71e+15*(T_300)^3.50*EXP(-12530.0/TK), b[M],0.60) ;
R[CI17]= CL + CLONO2 ----> CL2 + NO3    @ 6.20e-12*EXP(145.0/TK) ;
R[CI18]= CLO + HO2 ----> HOCL    @ 2.20e-12*EXP(340.0/TK) ;
NAMES
 PhotoRateIDs += {HOCL-06};
R[CI19]= HOCL -hv-> OH + CL    @ j[HOCL-06] ;
R[CI20]= CLO + CLO ----> 0.29*CL2 + 1.42*CL    @ 1.25e-11*EXP(-1960.0/TK) ;
R[CI21]= OH + HCL ----> CL    @ 1.70e-12*EXP(-230.0/TK) ;
R[CI22]= CL + H2 ----> HCL + HO2    @ 3.90e-11*EXP(-2310.0/TK) ;
R[CP01]= HCHO + CL ----> HCL + HO2 + CO    @ 8.10e-11*EXP(-30.0/TK) ;
R[CP02]= CCHO + CL ----> HCL + MECO3    @ 8.00e-11 ;
R[CP03]= MEOH + CL ----> HCL + HCHO + HO2    @ 5.50e-11 ;
R[CP04]= RCHO + CL ----> HCL + 0.9*RCO3 + 0.1*RO2C + 0.1*xCCHO + 0.1*xCO + 0.1*xHO2 +
0.1*yROOH    @ 1.23e-10 ;
R[CP05]= ACETONE + CL ----> HCL + RO2C + xHCHO + xMECO3 + yROOH    @ 7.70e-11*EXP(-
1000.0/TK) ;
R[CP06]= MEK + CL ----> HCL + 0.975*RO2C + 0.039*RO2XC + 0.039*zRNO3 + 0.84*xHO2 +
0.085*xMECO3 + 0.036*xRCO3 + 0.065*xHCHO + 0.07*xCCHO + 0.84*xRCHO + yROOH + 0.763*XC
@ 3.60e-11 ;
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R[CP07]= RNO3 + CL ----> HCL + 0.038*NO2 + 0.055*HO2 + 1.282*RO2C + 0.202*RO2XC +
0.202*zRNO3 + 0.009*RCHO + 0.018*MEK + 0.012*PRD2 + 0.055*RNO3 + 0.159*xNO2 + 0.547*xHO2
+ 0.045*xHCHO + 0.3*xCCHO + 0.02*xRCHO + 0.003*xACETONE + 0.041*xMEK + 0.046*xPROD2 +
0.547*xRNO3 + 0.908*yR6OOH + 0.201*XN + 0.0*XC    @ 1.92e-10 ;
R[CP08]= PRD2 + CL ----> HCL + 0.314*HO2 + 0.68*RO2C + 0.116*RO2XC + 0.116*zRNO3 +
0.198*RCHO + 0.116*PRD2 + 0.541*xHO2 + 0.007*xMECO3 + 0.022*xRCO3 + 0.237*xHCHO +
0.109*xCCHO + 0.591*xRCHO + 0.051*xMEK + 0.04*xPROD2 + 0.686*yR6OOH + 1.262*XC    @ 2.00e-
10 ;
R[CP09]= GLY + CL ----> HCL + 0.63*HO2 + 1.26*CO + 0.37*RCO3 + 0.0*XC    @ 8.10e-11*EXP(-
30.0/TK) ;
R[CP10]= MGLY + CL ----> HCL + CO + MECO3    @ 8.00e-11 ;
R[CP11]= CRES + CL ----> HCL + xHO2 + xBALD + yR6OOH    @ 6.20e-11 ;
R[CP12]= BALD + CL ----> HCL + BZCO3    @ 8.00e-11 ;
R[CP13]= ROOH + CL ----> HCL + 0.414*OH + 0.588*RO2C + 0.414*RCHO + 0.104*xOH + 0.482*xHO2
+ 0.106*xHCHO + 0.104*xCCHO + 0.197*xRCHO + 0.285*xMEK + 0.586*yROOH + 0.0*XC    @ 1.66e-
10 ;
R[CP14]= R6OOH + CL ----> HCL + 0.145*OH + 1.078*RO2C + 0.117*RO2XC + 0.117*zRNO3 +
0.145*PRD2 + 0.502*xOH + 0.237*xHO2 + 0.186*xCCHO + 0.676*xRCHO + 0.28*xPROD2 +
0.855*yR6OOH + 0.348*XC    @ 3.00e-10 ;
R[CP15]= RAOOH + CL ----> 0.404*HCL + 0.139*OH + 0.148*HO2 + 0.589*RO2C + 0.124*RO2XC +
0.124*zRNO3 + 0.074*PRD2 + 0.147*MGLY + 0.139*IPRD + 0.565*xHO2 + 0.024*xOH + 0.448*xRCHO
+ 0.026*xGLY + 0.03*xMEK + 0.252*xMGLY + 0.073*xAFG1 + 0.073*xAFG2 + 0.713*yR6OOH +
2.674*XC    @ 4.29e-10 ;
R[TP01]= ACROLEIN + CL ----> 0.484*xHO2 + 0.274*xCL + 0.216*MACO3 + 1.032*RO2C +
0.026*RO2XC + 0.026*zRNO3 + 0.216*HCL + 0.484*xCO + 0.274*xHCHO + 0.274*xGLY +
0.484*xCLCCHO + 0.784*yROOH + 0.0*XC    @ 2.94e-10 ;
R[CP16]= MACR + CL ----> 0.25*HCL + 0.165*MACO3 + 0.802*RO2C + 0.033*RO2XC + 0.033*zRNO3
+ 0.802*xHO2 + 0.541*xCO + 0.082*xIPRD + 0.18*xCLCCHO + 0.541*xCLACET + 0.835*yROOH +
0.208*XC    @ 3.85e-10 ;
R[CP17]= MVK + CL ----> 1.283*RO2C + 0.053*RO2XC + 0.053*zRNO3 + 0.322*xHO2 +
0.625*xMECO3 + 0.947*xCLCCHO + yROOH + 0.538*XC    @ 2.32e-10 ;
R[CP18]= IPRD + CL ----> 0.401*HCL + 0.084*HO2 + 0.154*MACO3 + 0.73*RO2C + 0.051*RO2XC +
0.051*zRNO3 + 0.042*AFG1 + 0.042*AFG2 + 0.712*xHO2 + 0.498*xCO + 0.195*xHCHO +
0.017*xMGLY + 0.009*xAFG1 + 0.009*xAFG2 + 0.115*xIPRD + 0.14*xCLCCHO + 0.42*xCLACET +
0.762*yR6OOH + 0.709*XC    @ 4.12e-10 ;
NAMES
 PhotoRateIDs += {CLCCHO};
R[CP19]= CLCCHO -hv-> HO2 + CO + RO2C + xCL + xHCHO + yROOH    @ j[CLCCHO] ;
R[CP20]= CLCCHO + OH ----> RCO3 + 0.0*XC    @ 3.10e-12 ;
R[CP21]= CLCCHO + CL ----> HCL + RCO3 + 0.0*XC    @ 1.29e-11 ;
NAMES
 PhotoRateIDs += {CLACET};
R[CP22]= CLACET -hv-> MECO3 + RO2C + xCL + xHCHO + yROOH    @5.00e-1 *  j[CLACET] ;
R[CP29]= xCL + NO ----> NO + CL    @ k[BR07] *1.0;
R[CP30]= xCL + HO2 ----> HO2    @ k[BR08] *1.0;
R[CP31]= xCL + NO3 ----> NO3 + CL    @ k[BR09] *1.0;
R[CP32]= xCL + MEO2 ----> MEO2 + 0.5*CL    @ k[BR10] *1.0;
R[CP33]= xCL + RO2C ----> RO2C + 0.5*CL    @ k[BR11] *1.0;
R[CP34]= xCL + RO2XC ----> RO2XC + 0.5*CL    @ k[BR11] *1.0;
R[CP35]= xCL + MECO3 ----> MECO3 + CL    @ k[BR25] *1.0;
R[CP36]= xCL + RCO3 ----> RCO3 + CL    @ k[BR25] *1.0;
R[CP37]= xCL + BZCO3 ----> BZCO3 + CL    @ k[BR25] *1.0;
R[CP38]= xCL + MACO3 ----> MACO3 + CL    @ k[BR25] *1.0;
R[CP39]= xCLCCHO + NO ----> NO + CLCCHO    @ k[BR07] *1.0;
R[CP40]= xCLCCHO + HO2 ----> HO2 + 2*XC    @ k[BR08] *1.0;
R[CP41]= xCLCCHO + NO3 ----> NO3 + CLCCHO    @ k[BR09] *1.0;
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R[CP42]= xCLCCHO + MEO2 ----> MEO2 + 0.5*CLCCHO + XC @ k[BR10] *1.0;
R[CP43]= xCLCCHO + RO2C ----> RO2C + 0.5*CLCCHO + XC @ k[BR11] *1.0;
R[CP44]= xCLCCHO + RO2XC ----> RO2XC + 0.5*CLCCHO + XC @ k[BR11] *1.0;
R[CP45]= xCLCCHO + MECO3 ----> MECO3 + CLCCHO @ k[BR25] *1.0;
R[CP46]= xCLCCHO + RCO3 ----> RCO3 + CLCCHO @ k[BR25] *1.0;
R[CP47]= xCLCCHO + BZCO3 ----> BZCO3 + CLCCHO @ k[BR25] *1.0;
R[CP48]= xCLCCHO + MACO3 ----> MACO3 + CLCCHO @ k[BR25] *1.0;
R[CP49]= xCLACET + NO ----> NO + CLACET @ k[BR07] *1.0;
R[CP50]= xCLACET + HO2 ----> HO2 + 3*XC @ k[BR08] *1.0;
R[CP51]= xCLACET + NO3 ----> NO3 + CLACET @ k[BR09] *1.0;
R[CP52]= xCLACET + MEO2 ----> MEO2 + 0.5*CLACET + 1.5*XC @ k[BR10] *1.0;
R[CP53]= xCLACET + RO2C ----> RO2C + 0.5*CLACET + 1.5*XC @ k[BR11] *1.0;
R[CP54]= xCLACET + RO2XC ----> RO2XC + 0.5*CLACET + 1.5*XC @ k[BR11] *1.0;
R[CP55]= xCLACET + MECO3 ----> MECO3 + CLACET @ k[BR25] *1.0;
R[CP56]= xCLACET + RCO3 ----> RCO3 + CLACET @ k[BR25] *1.0;
R[CP57]= xCLACET + BZCO3 ----> BZCO3 + CLACET @ k[BR25] *1.0;
R[CP58]= xCLACET + MACO3 ----> MACO3 + CLACET @ k[BR25] *1.0;
R[CE01]= CH4 + CL ----> HCL + MEO2 @ 7.30e-12*EXP(-1280.0/TK) ;
R[CE02]= ETHE + CL ----> xHO2 + 2*RO2C + xHCHO + CLCHO @ TROE(1.60e-29*(T_300)^-3.30,
3.10e-10*(T_300)^-1.00, b[M],0.60) ;
R[TE01]= PROPENE + CL ----> 0.124*HCL + 0.971*xHO2 + 0.971*RO2C + 0.029*RO2XC +
0.029*zRNO3 + 0.124*xACROLEIN + 0.306*xCLCCHO + 0.54*xCLACET + yROOH + 0.222*XC @
2.67e-10 ;
R[TE02]= BUTADIENE13 + CL ----> 0.39*xHO2 + 0.541*xCL + 1.884*RO2C + 0.069*RO2XC +
0.069*zRNO3 + 0.863*xHCHO + 0.457*xACROLEIN + 0.473*xIPRD + yROOH + 0.0*XC @ 4.90e-10 ;
R[CE03]= ISOP + CL ----> 0.15*HCL + 0.738*xHO2 + 0.177*xCL + 1.168*RO2C + 0.085*RO2XC +
0.085*zRNO3 + 0.275*xHCHO + 0.177*xMVK + 0.671*xIPRD + 0.067*xCLCCHO + yR6OOH + 0.018*XC
@ 4.80e-10 ;
R[TE03]= APIN + CL ----> 0.548*HCL + 0.252*xHO2 + 0.068*xCL + 0.034*xMECO3 + 0.05*xRCO3 +
0.016*xMACO3 + 2.258*RO2C + 0.582*RO2XC + 0.582*zRNO3 + 0.035*xCO + 0.158*xHCHO +
0.185*xRCHO + 0.274*xACETONE + 0.007*xGLY + 0.003*xBACL + 0.003*xMVK + 0.158*xIPRD +
0.006*xAFG1 + 0.006*xAFG2 + 0.001*xAFG3 + 0.109*xCLCCHO + yR6OOH + 3.543*XC @ 5.46e-10 ;
R[CE04]= ACYE + CL ----> HO2 + CO + XC @ TROE(5.20e-30*(T_300)^-2.40, 2.20e-10, b[M],0.60) ;
R[TE04]= TOLUENE + CL ----> 0.894*xHO2 + 0.894*RO2C + 0.106*RO2XC + 0.106*zRNO3 +
0.894*xBALD + 0.106*XC @ 6.20e-11 ;
R[TE05]= MXYL + CL ----> 0.864*xHO2 + 0.864*RO2C + 0.136*RO2XC + 0.136*zRNO3 + 0.864*xBALD
+ 1.136*XC @ 1.35e-10 ;
R[TE06]= OXYL + CL ----> 0.864*xHO2 + 0.864*RO2C + 0.136*RO2XC + 0.136*zRNO3 + 0.864*xBALD
+ 1.136*XC @ 1.40e-10 ;
R[TE07]= PXYL + CL ----> 0.864*xHO2 + 0.864*RO2C + 0.136*RO2XC + 0.136*zRNO3 + 0.864*xBALD
+ 1.136*XC @ 1.44e-10 ;
R[TE08]= TRIMETH + BENZ124 + CL ----> 0.838*xHO2 + 0.838*RO2C + 0.162*RO2XC + 0.162*zRNO3
+ 0.838*xBALD + 2.162*XC @ 2.42e-10 ;
R[TE09]= ETOH + CL ----> HCL + 0.688*HO2 + 0.312*xHO2 + 0.312*RO2C + 0.503*xHCHO +
0.688*CCHO + 0.061*xHOCCHO + 0.312*yROOH + 0.0*XC @ 8.60e-11*EXP(45.0/TK) ;
R[BC01]= ALK1 + CL ----> HCL + xHO2 + RO2C + xCCHO + yROOH @ 8.30e-11*EXP(-100.0/TK) ;
R[BC02]= ALK2 + CL ----> HCL + 0.97*xHO2 + 0.97*RO2C + 0.03*RO2XC + 0.03*zRNO3 +
0.482*xRCHO + 0.488*xACETONE + yROOH + 0.0*XC @ 1.20e-10*EXP(40.0/TK) ;
R[BC03]= ALK3 + CL ----> HCL + 0.835*xHO2 + 0.094*xTBUO + 1.361*RO2C + 0.07*RO2XC +
0.07*zRNO3 + 0.078*xHCHO + 0.34*xCCHO + 0.343*xRCHO + 0.075*xACETONE + 0.253*xMEK +
0.983*yROOH + 0.017*yR6OOH + 0.18*XC @ 1.86e-10 ;
R[BC04]= ALK4 + CL ----> HCL + 0.827*xHO2 + 0.003*xMEO2 + 0.004*xMECO3 + 1.737*RO2C +
0.165*RO2XC + 0.165*zRNO3 + 0.003*xCO + 0.034*xHCHO + 0.287*xCCHO + 0.412*xRCHO +
0.247*xACETONE + 0.076*xMEK + 0.13*xPROD2 + yR6OOH + 0.327*XC @ 2.63e-10 ;

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R[BC05]= ALK5 + CL ----> HCL + 0.647*xHO2 + 1.541*RO2C + 0.352*RO2XC + 0.352*zRNO3 +
0.022*xHCHO + 0.08*xCCHO + 0.258*xRCHO + 0.044*xACETONE + 0.041*xMEK + 0.378*xPROD2 +
yR6OOH + 2.368*XC    @ 4.21e-10 ;
R[BC06]= OLE1 + CL ----> 0.384*HCL + 0.873*xHO2 + 1.608*RO2C + 0.127*RO2XC + 0.127*zRNO3 +
0.036*xHCHO + 0.206*xCCHO + 0.072*xRCHO + 0.215*xACROLEIN + 0.019*xMVK + 0.038*xIPRD +
0.192*xCLCCHO + 0.337*xCLACET + 0.169*yROOH + 0.831*yR6OOH + 1.268*XC    @ 3.92e-10 ;
R[BC07]= OLE2 + CL ----> 0.279*HCL + 0.45*xHO2 + 0.442*xCL + 0.001*xMEO2 + 1.492*RO2C +
0.106*RO2XC + 0.106*zRNO3 + 0.19*xHCHO + 0.383*xCCHO + 0.317*xRCHO + 0.086*xACETONE +
0.042*xMEK + 0.025*xMACR + 0.058*xMVK + 0.161*xIPRD + 0.013*xCLCCHO + 0.191*xCLACET +
0.319*yROOH + 0.681*yR6OOH + 0.294*XC    @ 3.77e-10 ;
R[BC08]= ARO1 + CL ----> 0.84*xHO2 + 0.84*RO2C + 0.16*RO2XC + 0.16*zRNO3 + 0.84*xPROD2 +
XC    @ 2.16e-10 ;
R[BC09]= ARO2 + CL ----> 0.828*xHO2 + 0.828*RO2C + 0.172*RO2XC + 0.172*zRNO3 + 0.469*xBALD
+ 0.359*xPROD2 + 2.531*XC    @ 2.66e-10 ;
R[BC10]= TERP + CL ----> 0.548*HCL + 0.252*xHO2 + 0.068*xCL + 0.034*xMECO3 + 0.05*xRCO3 +
0.016*xMACO3 + 2.258*RO2C + 0.582*RO2XC + 0.582*zRNO3 + 0.035*xCO + 0.158*xHCHO +
0.185*xRCHO + 0.274*xACETONE + 0.007*xGLY + 0.003*xBACL + 0.003*xMVK + 0.158*xIPRD +
0.006*xAFG1 + 0.006*xAFG2 + 0.001*xAFG3 + 0.109*xCLCCHO + yR6OOH + 3.543*XC    @ 5.46e-10 ;
R[BC11]= SESQ + CL ----> 0.252*xHO2 + 0.068*xCL + 0.034*xMECO3 + 0.05*xRCO3 + 0.016*xMACO3
+ 2.258*RO2C + 0.582*RO2XC + 0.582*zRNO3 + 0.548*HCL + 0.035*xCO + 0.158*xHCHO +
0.185*xRCHO + 0.274*xACETONE + 0.007*xGLY + 0.003*xBACL + 0.003*xMVK + 0.158*xIPRD +
0.006*xAFG1 + 0.006*xAFG2 + 0.001*xAFG3 + 0.109*xCLCCHO + yR6OOH + 8.543*XC    @ k[BC10]
*1.0;
R[AE51]= BENZRO2 + NO ----> NO + BNZNRXN    @ k[BR07] *1.0;
R[AE52]= BENZRO2 + HO2 ----> HO2 + BNZHRXN    @ k[BR08] *1.0;
R[AE53]= XYLRO2 + NO ----> NO + XYLNRXN    @ k[BR07] *1.0;
R[AE54]= XYLRO2 + HO2 ----> HO2 + XYLHRXN    @ k[BR08] *1.0;
R[AE55]= TOLRO2 + NO ----> NO + TOLNRXN    @ k[BR07] *1.0;
R[AE56]= TOLRO2 + HO2 ----> HO2 + TOLHRXN    @ k[BR08] *1.0;
NAMES
 PhotoRateIDs += {HCHOR-06};
R[TR01]= HCHO + PRIMARY -hv->          @ j[HCHOR-06] ;
NAMES
 PhotoRateIDs += {HCHOM-06};
R[TR02]= HCHO + PRIMARY -hv->          @ j[HCHOM-06] ;
R[TR03]= HCHO + PRIMARY + OH ----> OH    @ 5.40e-12*EXP(135.0/TK) ;
R[TR05]= HCHO + PRIMARY + NO3 ----> NO3    @ 2.00e-12*EXP(-2431.0/TK) ;
R[TR06]= HCHO + PRIMARY + CL ----> CL    @ 8.10e-11*EXP(-30.0/TK) ;
R[TR07]= CCHO + PRIMARY + OH ----> OH    @ 4.40e-12*EXP(365.0/TK) ;
NAMES
 PhotoRateIDs += {CCHO_R};
R[TR08]= CCHO + PRIMARY -hv->          @ j[CCHO_R] ;
R[TR09]= CCHO + PRIMARY + NO3 ----> NO3    @ 1.40e-12*EXP(-1860.0/TK) ;
R[TR10]= CCHO + PRIMARY + CL ----> HCL    @ 8.00e-11 ;
R[TR11]= ACROLEIN + PRIMARY + OH ----> OH    @ 1.99e-11 ;
R[TR12]= ACROLEIN + PRIMARY + O3 ----> O3    @ 1.40e-15*EXP(-2528.0/TK) ;
R[TR13]= ACROLEIN + PRIMARY + NO3 ----> NO3    @ 1.18e-15 ;
R[TR14]= ACROLEIN + PRIMARY + O3P ----> O3P    @ 2.37e-12 ;
NAMES
 PhotoRateIDs += {ACRO-09};
R[TR15]= ACROLEIN + PRIMARY -hv->          @ j[ACRO-09] ;
R[TR16]= ACROLEIN + PRIMARY + CL ----> CL    @ 2.94e-10 ;*/
R[IS1]= ISOP + OH ----> ISOPO2 + ISOPRXN    @ 2.54e-11*EXP(410.0/TK) ;
R[IS2]= ISOPO2 + NO ----> 0.43*MVK + 0.28*MACR + 0.94*NO2 + 0.036*ISOPND + 0.024*ISOPNB +
0.7*HCHO + 0.11*HC5 + 0.046*ARO2 + 0.085*DIBOO + 0.85*HO2 + 0.0*XC   @ 2.60e-
12*EXP(380.0/TK) ;
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R[IS3]= ISOPO2 + HO2 ----> 0.880*ISOPOOH + 0.120*OH + 0.047*MACR + 0.073*MVK + 0.120*HO2 + 0.120*HCHO @ 2.06e-13*EXP(1300.0/TK) ;
R[IS4]= ISOPO2 + MEO2 ----> 0.45*HO2 + 0.37*HCHO + 0.23*MVK + 0.15*MACR + 0.05*DIBOO + 0.06*HC5 + 0.02*ARO2 + 0.5*PRD2 + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH + 0.0*XC @ 1.80e-12 ;
R[IS5]= ISOPO2 + RO2C ----> 0.45*HO2 + 0.37*HCHO + 0.23*MVK + 0.15*MACR + 0.05*DIBOO + 0.06*HC5 + 0.02*ARO2 + 0.5*PRD2 + 0.0*XC @ 6.80e-13 ;
R[IS6]= ISOPO2 + ISOPO2 ----> 0.91*HO2 + 0.75*HCHO + 0.45*MVK + 0.29*MACR + 0.09*DIBOO + 0.11*HC5 + 0.05*ARO2 + PRD2 + 0.0*XC @ 2.30e-12 ;
R[IS7]= ISOPO2 + MECO3 ----> MEO2 + CO2 + 0.91*HO2 + 0.75*HCHO + 0.45*MVK + 0.29*MACR + 0.09*DIBOO + 0.11*HC5 + 0.05*ARO2 + 0.0*XC @ 4.4e-13*EXP(1070.0/TK) ;

R[IS9]= ISOP + NO3 ----> NISOPO2 @ 3.03e-12*EXP(-448.0/TK) ;
R[IS10]= NISOPO2 + NO3 ----> 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 1.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5 @ 2.3e-12 ;
R[IS11]= NISOPO2 + NO ----> 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 1.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5 @ 2.60e-12*EXP(380.0/TK) ;
R[IS12]= NISOPO2 + HO2 ----> NISOPOOH @ 2.06e-13*EXP(1300.0/TK) ;
R[IS13]= NISOPO2 + MEO2 ----> 0.35*NIT1 + 0.0175*MVK + 0.0175*MACR + 0.15*NO2 + 0.40*HO2 + 0.035*HCHO + 0.115*HC5 + 0.25*NIT1 + 0.25*ISOPND + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH @ 1.3e-12 ;
R[IS14]= NISOPO2 + RO2C ----> 0.35*NIT1 + 0.0175*MVK + 0.0175*MACR + 0.15*NO2 + 0.40*HO2 + 0.035*HCHO + 0.115*HC5 + 0.25*NIT1 + 0.25*ISOPND @ 6.04e-13 ;
R[IS15]= NISOPO2 + MECO3 ----> MEO2 + CO2 + 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 0.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5 @ 4.4e-13*EXP(1070.0/TK) ;

R[IS17]= HC5 + OH ----> HC5OO @ 1.42e-11*EXP(610.0/TK) ;
R[IS18]= HC5OO + NO ----> NO2 + 0.234*HOCCHO + 0.234*MGLY + 0.216*GLY + 0.216*HACET + 0.29*DHMOB + 0.17*RCOOH + 0.09*PRD2 + 0.09*CO + HO2 + 0.16*XC @ 2.60e-12*EXP(380.0/TK) ;
R[IS19]= HC5OO + HO2 ----> R6OOH + 0.0*XC @ 2.06e-13*EXP(1300.0/TK) ;
R[IS20]= HC5OO + MEO2 ----> 0.117*HOCCHO + 0.117*MGLY + 0.108*GLY + 0.108*HACET + 0.145*DHMOB + 0.085*RCOOH + 0.045*PRD2 + 0.045*CO + 0.5*HO2 + 0.5*PRD2 + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO + 0.0*XC @ 2.0e-13 ;
R[IS21]= HC5OO + RO2C ----> 0.117*HOCCHO + 0.117*MGLY + 0.108*GLY + 0.108*HACET + 0.145*DHMOB + 0.085*RCOOH + 0.045*PRD2 + 0.045*CO + 0.5*HO2 + 0.5*PRD2 + 0.0*XC @ 3.50e-14 ;
R[IS22]= HC5OO + MECO3 ----> MEO2 + CO2 + 0.234*HOCCHO + 0.234*MGLY + 0.216*GLY + 0.216*HACET + 0.29*DHMOB + 0.17*RCOOH + 0.09*PRD2 + 0.09*CO + HO2 + 0.16*XC @ 4.4e-13*EXP(1070.0/TK) ;

R[IS24]= HC5 + O3 ----> 0.50*MGLY + 0.35*GLY + 0.79*OH + 0.02*HCHO + 0.35*HOCCHO + 0.59*CO + 0.15*HACET + 0.13*RCOOH + 0.08*CO2 + 0.6*HO2 + 0.35*MECO3 + 0.0*XC @ 3.94e-15*EXP(-1520.0/TK) ;
R[IS25]= ISOPND + OH ----> ISOPNOOD @ 2.40e-11*EXP(410.0/TK) ;
R[IS26]= ISOPNOOD + NO ----> 0.34*PRD2 + 0.15*PROPNN + 0.44*HACET + 0.07*MVKN + 0.13*ETHLN + 0.31*HCOOH + 0.31*NO3 + 0.72*HCHO + 0.15*HOCCHO + 1.34*NO2 + 0.35*HO2 + 0.0*XC @ 2.60e-12*EXP(380.0/TK) ;
R[IS27]= ISOPND + O3 ----> 0.36*ETHLN + 0.29*PROPNN + 0.70*MGLY + 0.12*RCOOH + 0.39*HO2 + 0.038*HCHO + 0.029*CO + 0.73*OH + 0.017*CO2 + 0.36*NO2 + 0.16*HACET + 0.34*HOCCHO + 0.0*XC @ 8.70e-15*EXP(-1520.0/TK) ;
R[IS28]= ISOPNB + OH ----> ISOPNOOB @ 3.28e-12*EXP(410.0/TK) ;
R[IS29]= ISOPNOOB + NO ----> 0.6*HOCCHO + 0.6*HACET + 0.4*HCHO + 0.4*HO2 + 0.26*MACRN + 0.14*MVKN + 1.6*NO2 @ 2.60e-12*EXP(380.0/TK) ;
R[IS30]= ISOPNB + O3 ----> 0.12*MVKN + 0.32*MACRN + 0.34*OH + 0.08*HO2 + 0.26*CO + 0.07*CO2 + 0.16*HCOOH + 0.56*HCHO + 0.28*RNO3I + 0.04*HACET + 0.28*NO2 + 0.24*BACL + 0.0*XC @ 2.13e-14*EXP(-1520.0/TK) ;

R[IS31]= NIT1 + NO3 ----> 0.6*NIT1NO3OOA + 0.6*HNO3 + 0.4*NIT1NO3OOB @ 3.15e-13*EXP(-448.0/TK) ;
R[IS32]= NIT1NO3OOA + NO3 ----> NO2 + PROPNNB + CO + CO2 + HO2 @ 4.0e-12 ;
R[IS33]= NIT1NO3OOB + NO3 ----> PROPNNB + GLY + NO2 + NO2 @ 2.3e-12 ;
R[IS34]= NIT1NO3OOA + NO ----> NO2 + PROPNNB + CO + CO2 + HO2 @ k[BR31] *1.0 ;
R[IS35]= NIT1NO3OOB + NO ----> 0.5*PROPNNB + 0.5*GLY + 0.5*NO2 + 0.5*RNO3I + 0.5*HCHO + 0.5*NO2 + NO2 + 0.0*XC @ 2.26e-12*EXP(380.0/TK) ;
R[IS36]= NIT1NO3OOA + HO2 ----> 0.75*RCOOOH + 0.25*RCOOH + 0.25*O3 + XN + 2*XC @ k[BR22] *1.0 ;
R[IS37]= NIT1NO3OOB + HO2 ----> RNO3I + XN + 0.0*XC @ 2.06e-13*EXP(1300.0/TK) ;
R[IS38]= NIT1NO3OOA + RO2C ----> PROPNNB + CO + CO2 + HO2 @ k[BR25] *1.0 ;
R[IS39]= NIT1NO3OOB + RO2C ----> 0.7*PROPNNB + 0.7*GLY + 0.7*NO2 + 0.3*RNO3I + 0.3*XN + 0.0*XC @ 3.50e-14 ;
R[IS40]= NIT1NO3OOA + MEO2 ----> PROPNNB + CO + CO2 + HO2 + HCHO + HO2 @ k[BR24] *1.0 ;
R[IS41]= NIT1NO3OOA + MECO3 ----> MEO2 + CO2 + PROPNNB + CO + CO2 + HO2 @ k[BR27] *1.0 ;

R[IS43]= NIT1NO3OOB + MEO2 ----> 0.7*PROPNNB + 0.7*GLY + 0.7*NO2 + 0.3*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.5*HCHO + 0.5*HO2 + 0.3*XN + 0.0*XC @ 2.0e-13 ;
R[IS44]= NIT1NO3OOB + MECO3 ----> MEO2 + CO2 + PROPNNB + GLY + NO2 @ 4.4e-13*EXP(1070.0/TK) ;

R[IS46]= NIT1 + O3 ----> 0.3*PROPNNB + 0.45*CO + 0.15*OH + 0.45*HO2 + 0.15*CO2 + 0.7*GLY + 0.7*OH + 0.7*NO2 + 0.7*MGLY @ 4.15e-15*EXP(-1520.0/TK) ;
R[IS47]= NIT1 + OH ----> 0.345*NIT1NO3OOA + 0.655*NIT1OHOO @ 7.48e-12*EXP(410.0/TK) ;
R[IS48]= NIT1OHOO + NO ----> 0.919*PROPNNB + 0.919*GLY + 0.015*CO + 0.015*RNO3I + 0.934*NO2 + 0.934*HO2 + 0.066*RNO3I + 0.0*XC + 0.066*XN @ 2.60e-12*EXP(380.0/TK) ;
R[IS50]= NIT1OHOO + HO2 ----> R6OOH + XN + 0.0*XC @ 2.06e-13*EXP(1300.0/TK) ;
R[IS51]= NIT1OHOO + RO2C ----> 0.689*PROPNNB + 0.689*GLY + 0.011*CO + 0.011*RNO3I + 0.7*HO2 + 0.3*RNO3I + 0.0*XC @ 3.5e-14 ;
R[IS52]= NIT1OHOO + MEO2 ----> 0.689*PROPNNB + 0.689*GLY + 0.011*CO + 0.011*RNO3I + 0.7*HO2 + 0.3*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.50*HCHO + 0.50*HO2 + 0.0*XC @ 2.0e-13 ;
R[IS53]= NIT1OHOO + MECO3 ----> MEO2 + CO2 + 0.984*PROPNNB + 0.984*GLY + 0.016*CO + 0.016*RNO3I + HO2 + 0.0*XC @ 4.4e-13*EXP(1070.0/TK) ;

R[IS55]= DIBOO + NO ----> NO2 + HO2 + 0.52*HOCCHO + 0.52*MGLY + 0.48*GLY + 0.48*HACET @ 2.60e-12*EXP(380.0/TK) ;
R[IS56]= MVK + OH ----> MVKOO @ 2.60e-12*EXP(610.0/TK) ;
R[IS57]= MVKOO + NO ----> 0.625*HOCCHO + 0.625*MECO3 + 0.265*MGLY + 0.265*HCHO + 0.265*HO2 + 0.11*MVKN + 0.89*NO2 @ 2.60e-12*EXP(380.0/TK) ;
R[IS58]= MVKOO + HO2 ----> ROOH + XC @ 1.82e-13*EXP(1300.0/TK) ;
R[IS59]= MVKOO + MEO2 ----> 0.35*HOCCHO + 0.35*MECO3 + 0.15*MGLY + 0.15*HCHO + 0.15*HO2 + 0.5*MEK + 0.25*HCHO + 0.25*MEOH + 0.5*HCHO + 0.50*HO2 @ 2.0e-13 ;
R[IS60]= MVKOO + RO2C ----> 0.15*HO2 + 0.15*HCHO + 0.35*MECO3 + 0.35*HOCCHO + 0.15*MGLY + 0.5*MEK @ 3.50e-14 ;
R[IS61]= MVKOO + MECO3 ----> MEO2 + CO2 + 0.3*HO2 + 0.3*HCHO + 0.7*MECO3 + 0.7*HOCCHO + 0.3*MGLY @ 4.4e-13*EXP(1070.0/TK) ;

R[IS00]= MACR + OH ----> 0.47*MACROO + 0.53*MACO3 @ 8.0e-12*EXP(380.0/TK) ;
R[IS63]= MACROO + NO ----> 0.85*NO2 + 0.85*HO2 + 0.72*HACET + 0.72*CO + 0.13*HCHO + 0.13*MGLY + 0.15*MACRN @ 2.60e-12*EXP(380.0/TK) ;
R[IS64]= MACROO + HO2 ----> ROOH + XC @ 1.82e-13*EXP(1300.0/TK) ;
R[IS65]= MACROO + MEO2 ----> 0.50*HO2 + 0.424*HACET + 0.424*CO + 0.076*HCHO + 0.076*MGLY + 0.5*PRD2 + 0.25*HCHO + 0.25*MEOH + 0.5*HCHO + 0.5*HO2 + 0.0*XC @ 2.0e-13 ;
R[IS66]= MACROO + RO2C ----> 0.50*HO2 + 0.424*HACET + 0.424*CO + 0.076*HCHO + 0.076*MGLY + 0.5*PRD2 + 0.0*XC @ 3.50e-14 ;

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R[IS67]= MACROO + MECO3 ----> MEO2 + CO2 + HO2 + 0.15*MGLY + 0.85*HACET + 0.85*CO +
0.15*HCHO    @ 4.4e-13*EXP(1070.0/TK) ;

R[IS69]= MACO3 + NO ----> NO2 + CO + CO2 + HCHO + MEO2    @ 6.70e-12*EXP(340.0/TK) ;
R[IS70]= MACO3 + HO2 ----> 0.75*RCOOOH + 0.25*RCOOH + 0.25*O3 + XC    @ k[BR22] *1.0;
R[IS71]= MACO3 + NO3 ----> NO2 + CO + CO2 + HCHO + MEO2    @ 4.0e-12 ;
R[IS72]= MACO3 + MEO2 ----> HCHO + HO2 + CO + CO2 + HCHO + MEO2    @ k[BR24] *1.0;
R[IS73]= MACO3 + RO2C ----> CO + CO2 + HCHO + MEO2    @ k[BR25] *1.0;
R[IS74]= MACO3 + RO2XC ----> CO + CO2 + HCHO + MEO2    @ k[BR25] *1.0;
R[IS75]= MACO3 + MECO3 ----> CO2 + MEO2 + CO + CO2 + HCHO + MEO2    @ k[BR27] *1.0;
R[IS76]= MACO3 + RCO3 ----> CO + CO2 + HCHO + MEO2 + RO2C + xHO2 + yROOH + xCCHO +
CO2    @ k[BR27] *1.0;
R[IS77]= MACO3 + BZCO3 ----> CO + CO2 + HCHO + MEO2 + BZO + RO2C + CO2    @ k[BR27] *1.0;
R[IS78]= MACO3 + MACO3 ----> 2*CO + 2*CO2 + 2*HCHO + 2*MEO2    @ k[BR27] *1.0;
R[IS79]= HOCCHO + OH ----> 0.75*HO2 + 0.25*OH + 0.13*GLY + 0.52*CO + 0.35*CO2 + 0.16*HCOOH
+ 0.71*HCHO    @ 0.8e-11 ;
R[IS80]= HACET + OH ----> 0.75*MGLY + 0.825*HO2 + 0.125*HCOOH + 0.1*OH + 0.125*MEO2 +
0.20*CO2 + 0.05*CO + 0.125*CCOOH    @ 2.15e-12*EXP(305.0/TK) ;
R[IS81]= HACET -hv-> HO2 + MECO3 + HCHO    @1.75e-1 *  j[C2COC_to_RO2] ;
R[IS82]= ETHLN + OH ----> HCHO + CO2 + NO2    @ 2.94e-12*EXP(365.0/TK) ;
R[IS83]= PROPNN + OH ----> MGLY + NO2    @ 4.0e-13 ;
R[IS93]= PROPNNB + OH ----> MGLY + NO2    @ 4.0e-13 ;
NAMES
 PhotoRateIDs += {NOA_to_Prds};
R[IS97]= PROPNN -hv-> MECO3 + HCHO + NO2    @ j[NOA_to_Prds] ;
R[IS98]= PROPNNB -hv-> MECO3 + HCHO + NO2    @ j[NOA_to_Prds] ;
R[IS84]= MVKN + OH ----> 0.65*HCOOH + 0.65*MGLY + 0.35*HCHO + 0.35*PYRUACD + NO3    @
3.5e-12*EXP(140.0/TK) ;
//R[IS105a]= MVKN -hv-> MECO3 + NO2 + HOCCHO    @ j[IC3ONO2_to_NO2] ;
R[IS85]= MACRN + OH ----> 0.08*CCOOH + 0.08*HCHO + 0.08*NO3 + 0.07*HCOOH + 0.07*NO3 +
0.07*MGLY + 0.85*HACET + 0.85*NO2 + 0.93*CO2    @ 1.28e-11*EXP(405.0/TK) ;
R[IS86]= DHMOB + OH ----> 1.5*CO + 0.5*HO2 + 0.5*HACET + 0.5*PRD2 + 0.0*XC    @ 1.0e-11 ;
R[IS87]= PYRUACD -hv-> CCHO + CO2    @ j[MGLY_to_HO2] ;
R[IS88]= ISOPOOH + OH ----> IEPOX + OH    @ 1.9e-11*EXP(390.0/TK) ;
R[IS89]= ISOPOOH + OH ----> 0.387*ISOPO2 + 0.613*HC5 + 0.613*OH    @ 4.75e-12*EXP(200.0/TK) ;
R[IS90]= IEPOX + OH ----> IEPOXOO    @ 5.78e-11*EXP(-400.0/TK) ;
R[IS91]= IEPOXOO + HO2 ----> 0.725*HACET + 0.275*HOCCHO + 0.275*GLY + 0.275*MGLY +
1.125*OH + 0.825*HO2 + 0.200*CO2 + 0.375*HCHO + 0.074*HCOOH + 0.251*CO    @ 2.06e-
13*EXP(1300.0/TK) ;
R[IS92]= ISOPOOH -hv-> OH + 0.91*HO2 + 0.75*HCHO + 0.45*MVK + 0.29*MACR + 0.11*HC5 +
0.09*DIBOO + 0.05*ARO2 + 0.0*XC   @ j[COOH_to_HO2] ;
R[IS96]= IEPOXOO + NO ----> 0.725*HACET + 0.275*HOCCHO + 0.275*GLY + 0.275*MGLY +
0.125*OH + 0.825*HO2 + 0.200*CO2 + 0.375*HCHO + 0.074*HCOOH + 0.251*CO + NO2    @ 2.26e-
12*EXP(380.0/TK) ;

R[IS94]= RNO3I + OH ----> NO2 + HO2 + PRD2    @ 8.00e-12 ;

R[IS99]= NISOPOOH + OH ----> RNO3I + OH   @ 5.0e-11 ;
// !R[IS100]= NC4CO3H + OH ----> NIT1NO3OOA    @ 2.52e-11 ; COMMENTED OUT OF
mech_SAPRC07TC_AE5_AQ_isoprene_v4_Sep_11.txt
// !R[IS101]= NIT1OOH + OH ----> NIT1OHOO    @ 2.81e-11 ; COMMENTED OUT OF
mech_SAPRC07TC_AE5_AQ_isoprene_v4_Sep_11.txt
R[IS102]= DIBOO + HO2 ---->  R6OOH + 0.0*XC    @ 2.06e-13*EXP(1300/TK) ;
R[IS103]= DIBOO + MEO2 ----> 0.5*HO2 + 0.26*HOCCHO + 0.26*MGLY + 0.24*GLY + 0.24*HACET +
0.5*PRD2 + 0.25*HCHO + 0.25*MEOH + 0.5*HCHO + 0.50*HO2 + 0.0*XC    @ 2.00e-13 ;
```

R[IS104]= DIBOO + RO2C ----> 0.5*HO2 + 0.26*HOCCHO + 0.26*MGLY + 0.24*GLY + 0.24*HACET + 0.5*PRD2 + 0.0*XC @ 3.50e-14 ;
R[IS105]= DIBOO + MECO3 ----> HO2 + 0.52*HOCCHO + 0.52*MGLY + 0.48*GLY + 0.48*HACET + MEO2 + CO2 @ 4.40e-13*EXP(1070/TK) ;
R[IS106]= MVKN -hv-> MECO3 + NO2 + HOCCHO @ j[NOA_to_Prds] ;
R[IS107]= ISOPO2 ----> HO2 + HPALD @ 4.07e+8*EXP(-7694/TK) ;
R[IS108]= MAPAN + OH ----> HACET + CO + NO2 @ 2.90e-11 ;
R[IS109]= NIT1NO3OOA + NO2 ----> MAPAN + XN + XC @ k[BR28] *1.0;
R[IS110]= MACRN -hv-> HACET + NO2 + CO + HO2 @ j[NOA_to_Prds] ;
R[IS111]= ETHLN -hv-> NO2 + HCHO + HO2 + CO @ j[NOA_to_Prds] ;
R[IS112]= IEPOXOO + MEO2 ----> 0.363*HACET + 0.138*HOCCHO + 0.138*GLY + 0.138*MGLY + 0.063*OH + 0.413*HO2 + 0.100*CO2 + 0.188*HCHO + 0.037*HCOOH + 0.126*CO + 0.5*PRD2 + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH + 0.0*XC @ 2.00e-13 ;
R[IS113]= IEPOXOO + RO2C ----> 0.363*HACET + 0.138*HOCCHO + 0.138*GLY + 0.138*MGLY + 0.063*OH + 0.413*HO2 + 0.100*CO2 + 0.188*HCHO + 0.037*HCOOH + 0.126*CO + 0.5*PRD2 + 0.0*XC @ 3.50e-14 ;
R[IS114]= IEPOXOO + MECO3 ----> 0.725*HACET + 0.275*HOCCHO + 0.275*GLY + 0.275*MGLY + 0.125*OH + 0.825*HO2 + 0.200*CO2 + 0.375*HCHO + 0.074*HCOOH + 0.251*CO + MEO2 + CO2 @ 4.40e-13*EXP(1070/TK) ;
// !<IS136> NC4CO2H + OH = PROPNNB + CO + HO2 # 2.16e-11; COMMENTED OUT OF mech_SAPRC07TC_AE5_AQ_isoprene_v4_Sep_11.txt
NAMES
PhotoRateIDs += {HPALD_to_Prds};
R[IS137]= HPALD -hv-> OH + HO2 + 0.5*HACET + 0.5*MGLY + 0.25*HOCCHO + 0.25*GLY + HCHO @ j[HPALD_to_Prds] ; // Peeters and Muller, 2010 PCCP
R[IS138]= HPALD + OH ----> OH + PRD2 + 0.0*XC @ 4.60e-11 ;
R[IS139]= NISOPOOH + OH ----> 0.3*NISOPO2 + 0.7*OH + 0.7*NIT1 @ 0.38e-11*EXP(200/TK) ;
R[IS140]= NISOPO2 + NISOPO2 ----> 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 0.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5 + 0.5*NIT1 + 0.5*ISOPND @ 1.20e-12 ;
R[IS141]= ISOPNOOD + HO2 ----> RNO3I + 0.0*XC @ 2.06e-13*EXP(1300/TK) ;
R[IS142]= ISOPNOOD + MEO2 ----> 0.17*PRD2 + 0.075*PROPNN + 0.22*HACET + 0.035*MVKN + 0.065*ETHLN + 0.155*HCOOH + 0.155*NO3 + 0.36*HCHO + 0.075*HOCCHO + 0.17*NO2 + 0.175*HO2 + 0.5*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO + 0.0*XC @ 2.00e-13 ;
R[IS143]= ISOPNOOD + RO2C ----> 0.17*PRD2 + 0.075*PROPNN + 0.22*HACET + 0.035*MVKN +0.065*ETHLN + 0.155*HCOOH + 0.155*NO3 + 0.36*HCHO + 0.075*HOCCHO + 0.17*NO2 + 0.175*HO2 + 0.5*RNO3I + 0.0*XC @ 3.50e-14 ;
R[IS144]= ISOPNOOD + MECO3 ----> MEO2 + CO2 + 0.34*PRD2 + 0.15*PROPNN + 0.44*HACET + 0.07*MVKN + 0.13*ETHLN + 0.31*HCOOH + 0.31*NO3 + 0.72*HCHO + 0.15*HOCCHO + 0.34*NO2 + 0.35*HO2 + 0.0*XC @ 4.40e-13*EXP(1070/TK) ;
R[IS145]= ISOPNOOB + HO2 ----> RNO3I + 0.0*XC @ 2.06e-13*EXP(1300/TK) ;
R[IS146]= ISOPNOOB + MEO2 ----> 0.3*HOCCHO + 0.3*HACET + 0.2*HCHO + 0.2*HO2 + 0.13*MACRN + 0.07*MVKN + 0.3*NO2 + 0.5*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO + 0.0*XC @ 2.00e-13 ;
R[IS147]= ISOPNOOB + RO2C ----> 0.3*HOCCHO + 0.3*HACET + 0.2*HCHO + 0.2*HO2 + 0.13*MACRN + 0.07*MVKN + 0.3*NO2 + 0.5*RNO3I + 0.0*XC @ 3.50e-14 ;
R[IS148]= ISOPNOOB + MECO3 ----> MEO2 + CO2 + 0.6*HOCCHO + 0.6*HACET + 0.4*HCHO + 0.4*HO2 + 0.26*MACRN + 0.14*MVKN + 0.6*NO2 @ 4.40e-13*EXP(1070/TK) ;

APPENDIX B: UNC AUXILIARY MECHANISM REACTIONS LISTING

```
/*****************************************************************************
*                                                                            *
*   UNC Chamber Dependent NOx + WH2O Reactions (Walls)                       *
*   Units are molecules/cc/secs                                              *
*                                                                            *
*****************************************************************************/

// ========================================================================
//                                NO2 wall water reactions
//
SCALAR
 sf_depoNO2f  = 1.0,
 sf_depoNO2r  = 1.0,
 sf_WH2OpWNO2 = 1.0;

 R[DepoNO2f ] =    NO2     + WH2O      ---->  WNO2         @ 2.00E-20 * sf_depoNO2f;
 R[DepoNO2r ] =             WNO2      ---->  HONO + WHNO3 @ 2.64E-5  * sf_depoNO2r;

 R[WNO2pWNO2] =    WNO2    + WNO2      ---->  WN2O4        @ 2.00E-15 * sf_WH2OpWNO2;
 R[WH2OpWN2O4]=    WN2O4   + WH2O      ---->  WHONO + WHNO3
                                                                  @ 4.00E-15 *
sf_WH2OpWNO2;

// ========================================================================
//                                  WHNO3 acid reactions
//
SCALARS
#select
 #case _WHNO3_f_
   sf_NO_WHNO3_src  = 1.0,
   sf_NO2WHNO3_src  = 1.0,
 #case _WHNO3_g_
   sf_NO_WHNO3_src  = 1.0,
   sf_NO2WHNO3_src  = 1.0,
 #case _WHNO3_h_
   sf_NO_WHNO3_src  = 0.0,
   sf_NO2WHNO3_src  = 0.0,
 #else
   sf_NO_WHNO3_src  = 1.0,
   sf_NO2WHNO3_src  = 1.0,
#end
 sf_NO2_wall_src  = 8.0E-5;   // scales NO2 photolysis rate

 R[WHNO3NO ]  =      NO  + WHNO3 ----> 1.0*HONO + 1.0*NO2  @ 6.09E-18 * sf_NO_WHNO3_src;
 R[WHNO3NO2]  =      NO2 + WHNO3 ----> 1.0*HONO + 1.0*NO2  @ 3.38E-19 * sf_NO2WHNO3_src;
 R[WHNO3hv ]  =           WHNO3 -hv-> NO2              @ j[NO2_to_O3P]
                                              * sf_NO2_wall_src ;

// ========================================================================
//                               light dependent HONO production
//
// Reverted to Old wall model
// sf_HONO_wall_src_expt = New scalar added to be modified in react files for particular
```

```
//                    experimental conditions only if needed
SCALARS
#select
#case _NO2hv_g_
  sf_HONO_wall_src_expt = 0.7;
#end

SCALARS
  sf_HONO_wall_src      = 0.2E-3;

 R[WNO2hvHONO] =          NO2   -hv-> HONO       @ j[NO2_to_O3P] *
                                  sf_HONO_wall_src_expt * sf_HONO_wall_src ;


#end   // UNCAUXNOXWALLS_G_RXN_


/*************************************************************************
*                                                                        *
*   UNC Chamber Dependent Inorganic Reactions (Std)                      *
*   Units are cm^3_molecule^-1_s^-1                                      *
*                                                                        *
*************************************************************************/

// this version has lower rates for
//  R[DepoHONOf] ,R[DepoHONOr]
//  R[DepoN2O5d] was added and k_depo_N2O5 was recomputed. -HEJ


// ======================================================================
//                                  H2O2 and O3 wall deposition
//
SCALAR
 k_depo_H2O2 = 6.7E-4, // measured  loss rate, 1/sec
 k_depo_O3   = 2.3E-6; // measured  loss rate, 1/sec (EUPHORE 3.0E-6 /sec)

 R[DepoH2O2] =       H2O2 ---->              @ k_depo_H2O2 ;
 R[DepoO3  ] =       O3   ---->              @ k_depo_O3   ;


// ======================================================================
//                              N2O5 wall deposition and hydrolysis

// The "dry" deposition of N2O5
//       k[DepoN2O5d] is measured by Tuazon 83

 R[DepoN2O5d] =         N2O5  ----> 2.0*WHNO3    @ 4.2E-5;

// The "wet" deposition of N2O5
SCALARS
 sf_WH2OpN2O5 = 1.0,
 k_depo_N2O5;

// k[DepoN2O5b] is 7.4E-5 /s at 300K
//  based on work of Wahner et al, GRL, 25(12):2169,1998
//   and emperical tests in NOx limited experiments
```

```
 withk k_depo_N2O5 = 9.0E-22*EXP(2000.0/TK);

 R[DepoN2O5] =  N2O5 + WH2O  ----> 2.0 * WHNO3  @ k_depo_N2O5 * sf_WH2OpN2O5 ;

// ===========================================================================
//                                    HNO3 wall partitioning
//
// EUPHORE first order dry rate was 8.2E-5 /sec
SCALAR
 sf_depo_HNO3f = 1.0,
 sf_depo_HNO3r = 1.0,
 sf_depo_HNO3l = 1.0;

 R[DepoHNO3f] =    HNO3 + WH2O   ----> WHNO3   @ 2.6E-18 * sf_depo_HNO3f ;
 R[DepoHNO3r] =          WHNO3  ----> HNO3    @ 6.6E-6  * sf_depo_HNO3r ;
 R[DepoHNO3l] =          WHNO3  ---->         @ 3.0E-6  * sf_depo_HNO3l ;


// ===========================================================================
//                                    HONO wall partitioning

SCALAR
#select
 #case _HONOdep_d_
   sf_depo_HONOf = 1.0,
   sf_depo_HONOr = 1.0;
 #case _HONOdep_e_
   sf_depo_HONOf = 0.0,
   sf_depo_HONOr = 0.0;
 #else
   sf_depo_HONOf = 1.0,
   sf_depo_HONOr = 1.0;
 #end

 R[DepoHONOf] =    HONO  + WH2O  ----> WHONO   @ 4.5E-21 * sf_depo_HONOf ;
                           //decreased from UNCAuxInorgStd_a.rxn
 R[DepoHONOr] =          WHONO  ----> HONO    @ 3.3E-3  * sf_depo_HONOr ;
                           //decreased from UNCAuxInorgStd_a.rxn


#end   // UNCAUXINORSTD_d_RXN_
```

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