Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical and experimental study of peroxy and alkoxy radicals in the NO_3-initiated oxidation of isoprene

— Electronic Supplementary Information —

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A. Initial NO_3 and O_2 addition on carbon C4 of isoprene

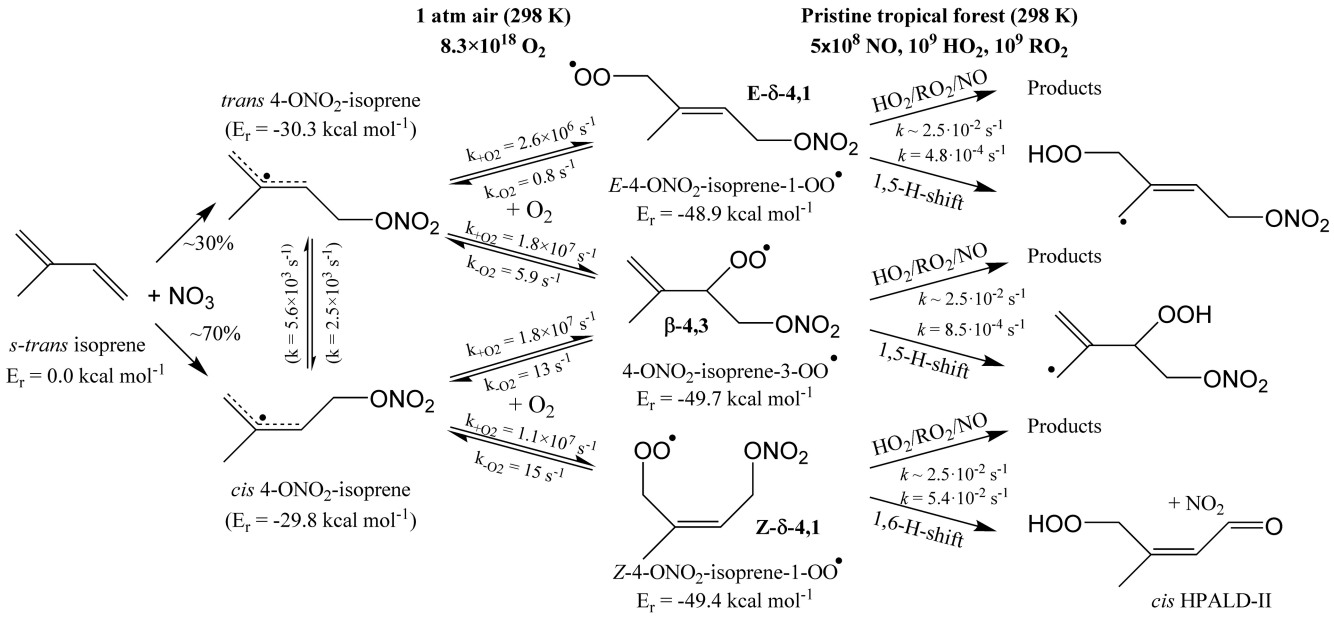

Figure S1: Reaction scheme for the site-specific addition of NO_3 on C4 of isoprene, and the subsequent stereo-specific addition of O_2. The co-reactant concentrations are taken as in Peeters et al.[1]

B. Initial NO_3 and O_2 addition on carbons C2 and C3 of isoprene

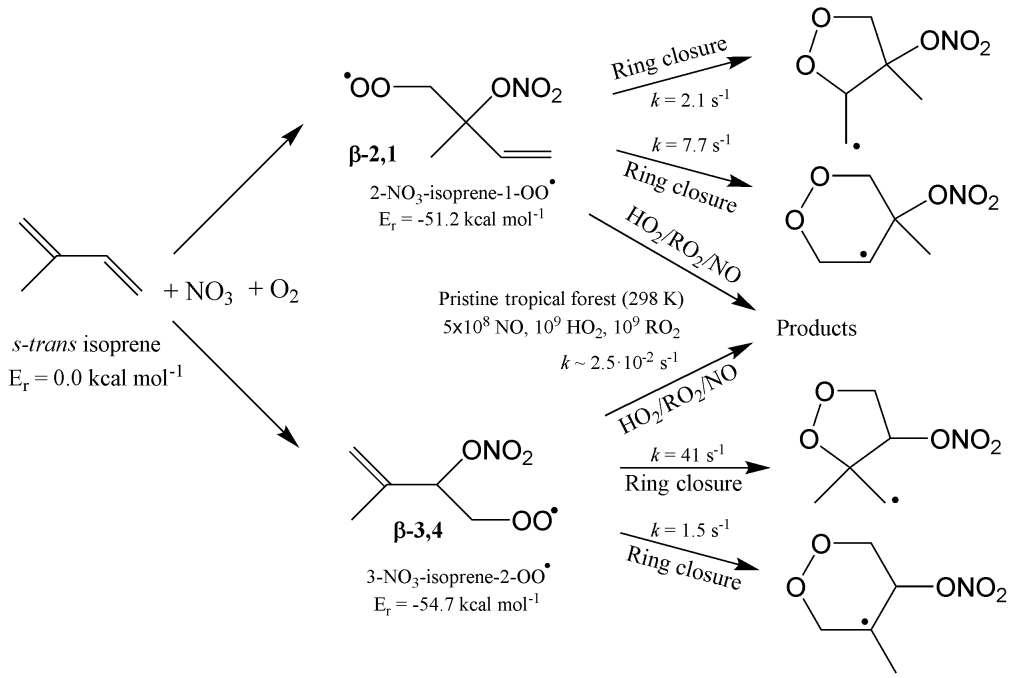

Figure S2: Reaction scheme for the site-specific addition of NO_3 on C2 and C3 of isoprene, and the subsequent addition of O_2. The co-reactant concentrations are taken as in Peeters et al.[1]

C. NO_3-isoprenyl and NO_3-isoprene-$OO^{\cdot}$ populations, and O_2 addition/elimination rate coefficients

The nascent NO_3-isoprenyl population is determined by the site-specificity of the NO_3 addition on the isoprene double bonds, followed by the collisional stabilisation of the resulting alkyl radicals. The site-specificity of the NO_3 addition is taken from the review by Wennberg et al., i.e. a ratio of 87:13 for addition to C1:C4, with addition to C2 and C3 currently disabled due to lack of data. Peeters et al.[1,2] and Dibble[3] analyzed the collisional stabilisation of the alkyl radicals formed in the addition of OH on isoprene, finding that internal rotation along the allylic bond is fast at the energies directly after OH addition, while at thermal energies the rotation is slow compared to other reactions. For C1-OH addition, the nascent distribution of cis- to trans-adducts was predicted to be about 5:5, while for C4-OH addition a ratio of 7:3 was found. In the NO_3-isoprenyl system, we feel that the addition energy and the barrier to internal rotation are sufficiently similar to the OH-isoprenyl system to assume similar nascent distributions, i.e. *C1-cis*:*C1-trans* = 1:1, and *C4-cis*:*C4-trans* = 7:3. As shown later, our experiments are not sensitive to this ratio.

No experimental data is available for the site-specific O_2 addition rates for the NO_3-isoprenyl radicals. A theoretical prediction of the rate coefficients is complex, as it requires characterization of the low and broad recombination reaction energy profile of the doublet allylic NO_3-isoprenyl radicals bonding with the triplet O_2 molecule. Due to spin contamination, multi-reference effects, and difficulties in describing the variational character of such near-barrierless transition states, theory-predicted rate coefficients are not expected to be overly accurate unless calculations are performed at a level of theory that is hard to attain for the current large molecules (11 non-hydrogen atoms). The predicted loss rates of the RO_2 radicals (see main text) suggests that for atmospheric conditions, or for the dilute conditions in the current set of experiments, the re-equilibration of the RO_2 radicals by O_2-elimination and re-addition is significantly faster than chemical loss processes. The RO_2 population should thus be close to the equilibrium distribution, and the exact values of the O_2 addition or elimination rate coefficients become less important. At this time, we therefore adopt O_2 addition rates similar as those used in the isoprene+OH system. The equilibrium constants obtained from the theoretical study of the alkyl and nitrate-RO_2 radicals then allow derivation of the reverse rate coefficients for O_2-elimination from the nitrate-RO_2.

$$K_{eq}(T)=\frac{[RO_2]}{[R][O_2]}=\frac{Q_{RO_2}(T)\exp\left(\frac{E_{R+O_2}-E_{RO_2}}{kT}\right)}{Q_R(T)Q_{O_2}(T)}=\frac{k_{R+O_2\rightarrow RO_2}(T)}{k_{RO_2\rightarrow R+O_2}(T)}$$

These rates will also guarantee that the system will evolve to the correct equilibrium population in the limit of negligible chemical losses; as discussed by Novelli et al.,[4] such balancing of O_2 addition and elimination rate constants is important to maintain the correct product distributions in this limit. Of the distinct sets of rate coefficients discussed in Novelli et al.,[4] we adopt the values for O_2 addition as used in the MCM v3.3.1[5] (see Table S1), which are based on the rate predictions by Peeters et al.[1,2] but calibrated against the absolute rate measurement for O_2 elimination by Teng et al.[6] Table S1 also lists the theory-derived equilibrium constants, and the resulting O_2 elimination rate constants for nitrate-RO_2 radicals. If updated values become available for any of the channels, the equilibrium constant can be used to re-balance the reverse reaction rate. From the data listed in Table S1 and the nascent NO_3-isoprenyl population one can then derive the nascent and equilibrium populations of the nitrate-RO_2 radicals from isoprene, These are listed in Table S2 for 298 K, and compared against examples of instantaneous populations in the experiments described in this work. They are also compared against the estimates of Schwantes et al.,[7] which are very different from our theory-based analysis.

Table S1: Rate coefficients $k_{forward}(T)$ for O_2 addition on NO_3-isoprene adducts, the equilibrium constants $K_{eq}(T)$, and the rate coefficient $k_{reverse}(T)$ for O_2 elimination from NO_3-isoprene-OO• radicals. Also listed are the equilibrium constant between cis- and trans-NO_3-isoprenyl. Indicated are the relative energy of the products E_{prod} (kcal mol^{-1}), estimated room temperature values (cm^3 molecule^{-1} s^{-1}, cm^3 molecule^{-1}, and s^{-1}, respectively), and the parameters of a Kooij expression, $k(220\text{-}450\ K) = A \times T^n \exp(-E_a/T)$. $k_{forward}(T)$ is obtained from the literature,[1,2,4,5] $K_{eq}(T)$ and $K_{reverse}(T)$ are obtained from that data and the theoretical characteristics.

Reactant(s)	**Product(s)**	E_{prod}	*Data*	**298 K**	*A*	*n*	E_a
trans-1-NO_3-isoprene	*cis*-1-NO_3-isoprene	0.99	K_{eq}(T)	2.1×10^{-1}	9.10E+00	-0.3	580
trans-1-NO_3-isoprene + O_2	*E*-1-NO_3-isoprene-4-OO•	-16.4	$k_{forward}$(T)	5×10^{-13}	2.5E-12		480
			K_{eq}(T)	1.0×10^{-14}	1.04E-27	0.40	-8227
			$k_{reverse}$(T)	5.0×10^{1}	2.40E+15	-0.40	8707
trans-1-NO_3-isoprene + O_2	1-NO_3-isoprene-2-OO•	-18.7	$k_{forward}$(T)	3.0×10^{-12}	3.0E-12		
			K_{eq}(T)	4.2×10^{-14}	6.41E-32	1.48	-9713
			$k_{reverse}$(T)	7.2×10^{1}	4.68E+19	-1.48	9713
cis-1-NO_3-isoprene + O_2	1-NO_3-isoprene-2-OO•	-19.7	$k_{forward}$(T)	3.0×10^{-12}	3.0E-12		
			K_{eq}(T)	2.0×10^{-13}	7.05E-33	1.80	-10293
			$k_{reverse}$(T)	1.5×10^{1}	4.26E+20	-1.80	10293
cis-1-NO_3-isoprene + O_2	*Z*-1-NO_3-isoprene-4-OO•	-18.4	$k_{forward}$(T)	3.5×10^{-12}	3.5E-12		
			K_{eq}(T)	2.1×10^{-14}	4.53E-36	2.94	-9870
			$k_{reverse}$(T)	1.7×10^{2}	7.72E+23	-2.94	9870
trans-4-NO_3-isoprene	*cis*-4-NO_3-isoprene	0.44	K_{eq}(T)	2.3×10^{0}	4.46E+00	0.07	324
trans-4-NO_3-isoprene + O_2	*E*-4-NO_3-isoprene-1-OO•	-18.6	$k_{forward}$(T)	5×10^{-13}	2.5E-12		480
			K_{eq}(T)	6.1×10^{-13}	3.11E-29	0.98	-9507
			$k_{reverse}$(T)	8.2×10^{-1}	8.05E+16	-0.98	9987
trans-4-NO_3-isoprene + O_2	4-NO_3-isoprene-3-OO•	-19.5	$k_{forward}$(T)	3.5×10^{-12}	3.5E-12		
			K_{eq}(T)	5.9×10^{-13}	6.20E-31	1.41	-9947
			$k_{reverse}$(T)	5.9×10^{0}	5.64E+18	-1.41	9947
cis-4-NO_3-isoprene + O_2	4-NO_3-isoprene-3-OO•	-19.9	$k_{forward}$(T)	3.5×10^{-12}	3.5E-12		
			K_{eq}(T)	2.6×10^{-13}	1.39E-31	1.34	-10271
			$k_{reverse}$(T)	1.3×10^{1}	2.51E+19	-1.34	10271
cis-4-NO_3-isoprene + O_2	*Z*-4-NO_3-isoprene-1-OO•	-19.6	$k_{forward}$(T)	2.0×10^{-12}	2.00E-12		
			K_{eq}(T)	1.3×10^{-13}	2.64E-35	2.74	-10238
			$k_{reverse}$(T)	1.5×10^{1}	7.58E+22	-2.74	10238

Table S2: Population contributions (fraction) at 298K for each of the ensembles of interchanging radical pools. Indicated are the nascent population and equilibrium population at 298 K, and a representative instantaneous population in each of the three experiments after approximately 1 hour of reaction time in the SAPHIR chamber (i.e. midway in the first injection period). Also shown are the data by Schwantes et al. derived from experimental product yields.

Intermediate	Nascent 298 K	Equilibrium 298 K	10 Aug 2018 301 K	12 Aug 2018 302 K	13 Aug 2018 297 K	Schwantes et al.[7]
trans-1-NO_3-isoprenyl	0.50	0.82	0.82	0.82	0.83	
cis-1-NO_3-isoprenyl	0.50	0.18	0.18	0.18	0.17	
E-1-NO_3-isoprene-4-$OO^\bullet$	0.05	0.18	0.18	0.19	0.18	E+Z: 0.44-0.46 [a]
1-NO_3-isoprene-2-$OO^\bullet$	0.60	0.74	0.75	0.75	0.76	0.42 [a]
Z-1-NO_3-isoprene-4-$OO^\bullet$	0.35	0.08	0.07	0.07	0.07	E+Z: 0.44-0.46 [a]
trans-4-NO_3-isoprenyl	0.30	0.33	0.31	0.30	0.31	
cis-4-NO_3-isoprenyl	0.70	0.70	0.69	0.70	0.69	
E-4-NO_3-isoprene-1-$OO^\bullet$	0.03	0.40	0.42	0.39	0.42	E+Z: 0.08-0.09 [a]
4-NO_3-isoprene-3-$OO^\bullet$	0.70	0.40	0.37	0.38	0.37	E+Z: 0.03-0.06 [a]
Z-4-NO_3-isoprene-1-$OO^\bullet$	0.27	0.20	0.21	0.22	0.21	E+Z: 0.08-0.09 [a]

[a] Overall distribution. As only ranges are given for most of the intermediates, these are not rescaled to fractions specific to the NO_3 addition site.

D. Oxidation scheme for *E*- and *Z*-1-ONO_2-isoprene-4-O• radicals

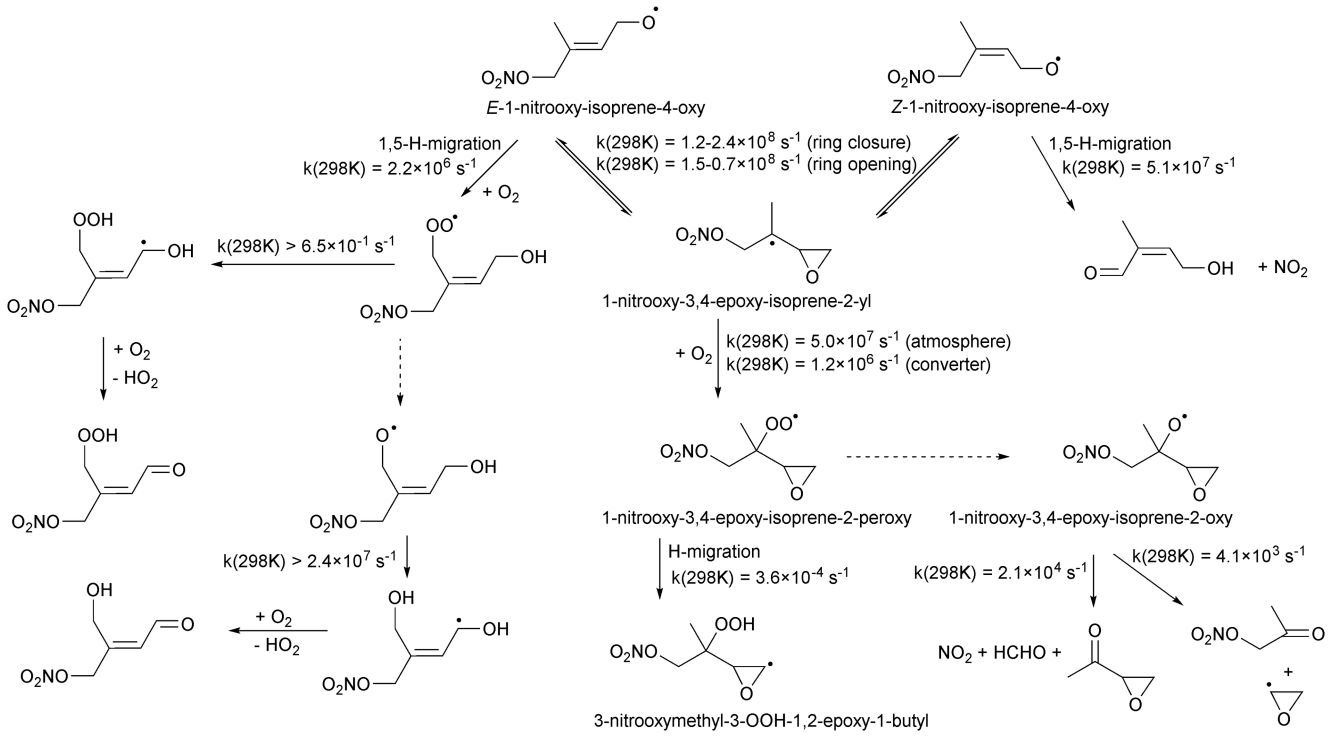

Figure S3: Reaction scheme for the dominant reaction pathways for 1-NO_3-isoprene-4-O• radicals. The dotted arrows indicates alkoxy radical formation in the reaction of RO_2 with NO, NO_3, HO_2, or $R'O_2$; these reactions are not depicted.

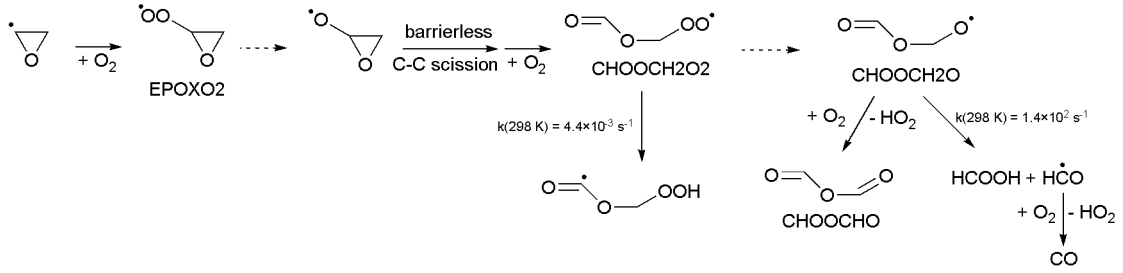

Figure S4: Reaction scheme for the dominant reaction pathways for the epoxy-ethyl radical degradation. The dotted arrow indicates alkoxy radical formation in the reaction of RO_2 with NO, NO_3, HO_2, or $R'O_2$; these reactions are not depicted. Our CCSD(T)//M06-2X calculations find a vanishingly low barrier for bond breaking in the epoxy-ethoxy radical, which becomes negative after ZPE-corrections, indicating a barrierless process. The rate coefficient for the 1,5-H-migration in the CHOOCH2O2 peroxy radical was calculated as k(200-450 K) = 1.16×10^{-83} $(T/K)^{30.46}$ exp(3585K/T), with a barrier of 22.6 kcal mol^{-1}.

E. Oxidation scheme for 4-ONO_2-isoprene-3-O• radicals

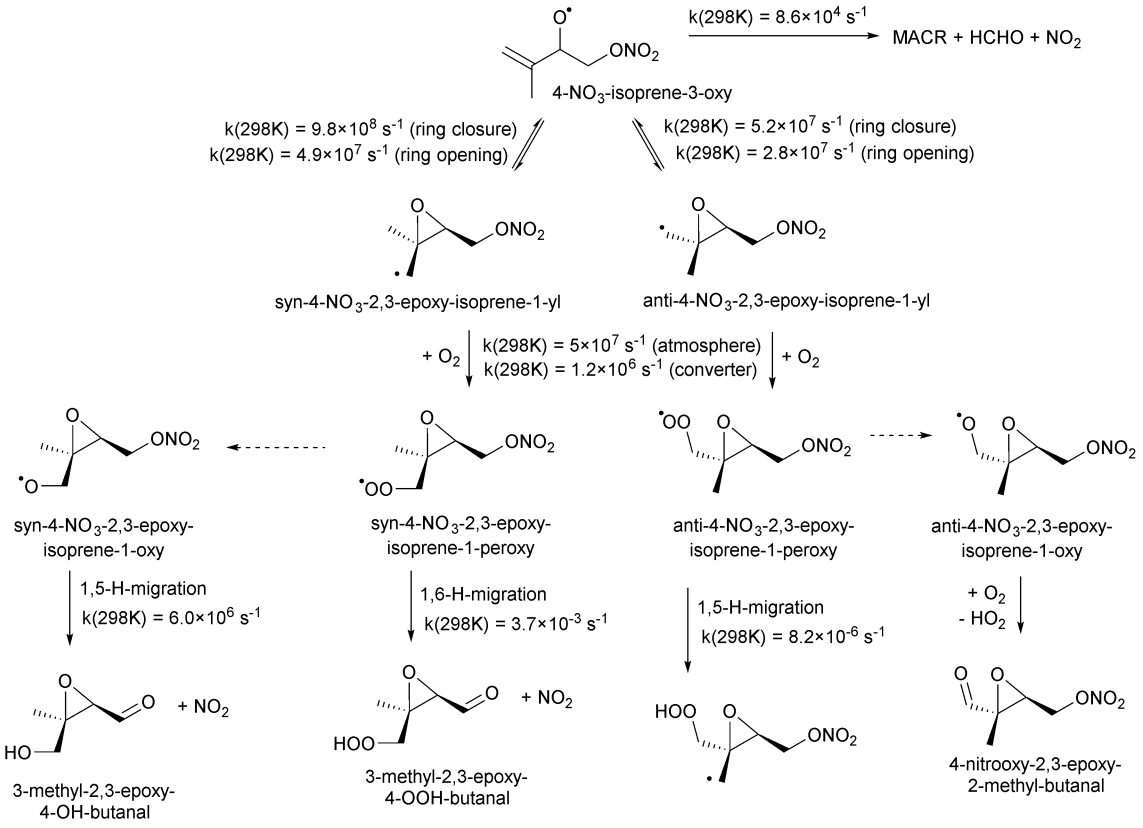

Figure S5: Reaction scheme for the dominant reaction pathways for 4-NO_3-isoprene-3-O• radicals. The dotted arrows indicates alkoxy radical formation in the reaction of RO_2 with NO, NO_3, HO_2, or R'O_2; these reactions are not depicted.

F. Oxidation scheme for *Z*- and *E*-4-ONO_2-isoprene-1-O• radicals

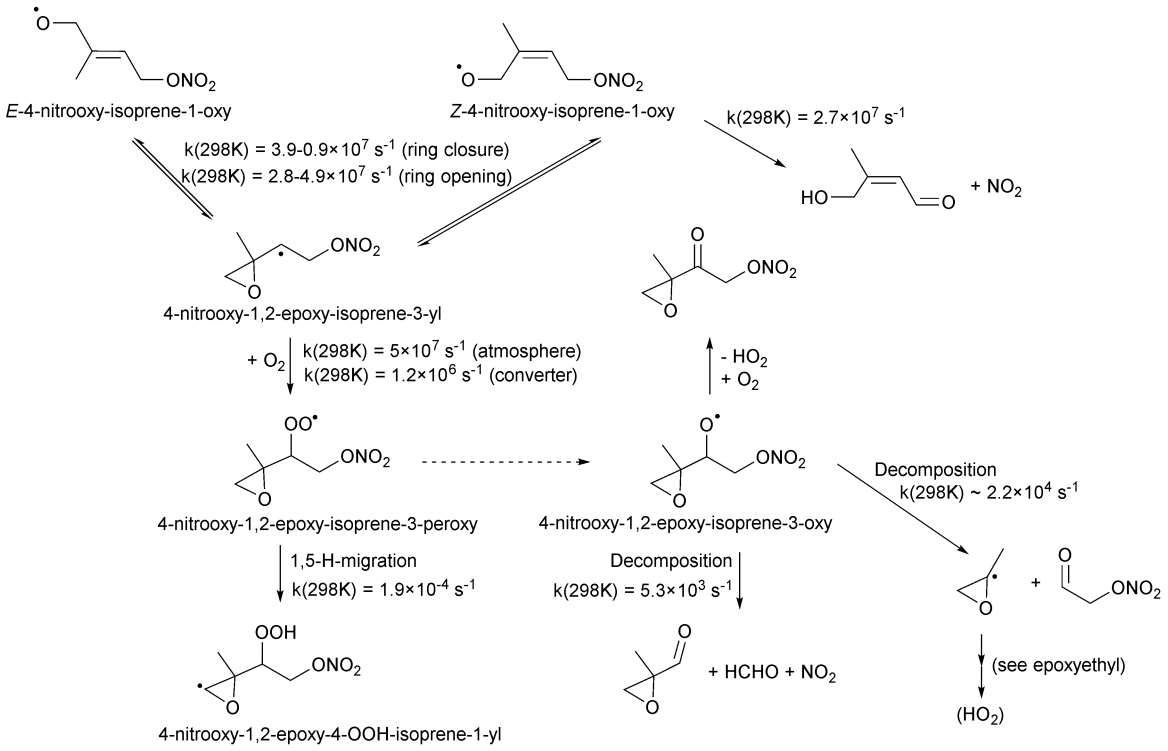

Figure S6: Reaction scheme for the dominant reaction pathways for 4-NO_3-isoprene-1-O• radicals. The dotted arrows indicates alkoxy radical formation in the reaction of RO_2 with NO, NO_3, HO_2, or R'O_2; these reactions are not depicted. By analogy with the epoxy-ethyl radical (Figure S4), we assume that the 1,2-epoxy-2-propyl radical can ultimately yield an HO_2 radical in the high-NO low-pressure reaction conditions of the converter.

G. Updating the isoprene ozonolysis scheme

For isoprene, we base the update mostly on the recent work by Wennberg et al.[8] and Nguyen et al.[9] For the *E*-RCHOO Criegee intermediates, we adopt a methacrylic acid yield of 5 %,[10] and assume a 2:1:1 ratio of formation of CO_2 and CO with recombination or radical co-products similar to that adopted for CH_2OO in Novelli et al.[11] Note that no ketene + H_2O channel is possible here due to the presence of a double bond; pyrolysis of methacrylic acid and other α-β-unsaturated acids proceeds mostly by decarboxylation to the alkene,[12] confirming our adoption here of an alkene as the main channel. Methylenol is not included in the MCM v3.3.1, so we invoke keto-enol isomerisation to use acetone as a product instead.

The theoretical study of Kuwata et al.[13,14] on MVK-oxide showed that the 1,5-ring closure forming cyclic alkeneperoxide is highly exothermic, such that the cyclic alkeneperoxide is not stabilized at 1 atm. and rearrange forming dicarbonyl and epoxides in a roughly 60:40 ratio. More recent works by Barber et al.[15] and Vansco et al.[16] surprisingly fail to mention the epoxide channel, but find that at low pressure (~10 Torr) the dicarbonyl compounds readily decompose by C–C bond scission, forming an acyl and vinoxy radical that react with O_2 and decompose again at low pressure. At 1 atm, though, they expect mostly stabilization of the peroxy radicals formed from the acyl and vinoxy radicals. What is less clear is to what extend the dicarbonyl intermediates are thermalized at 1 atm., given that the dissociation of these compounds proceeds through a channel only ~20 kcal mol^{-1} below the energy of the parent CI, following a very deep energy well at -95 kcal mol^{-1} that should lead to high state densities of the intermediate and thus low energy-specific dissociation rate coefficients k(E). As these channels are not overly important in our system, we adopt formation of stabilized carbonyls as the main fate at 1 atm, awaiting more information on the thermalization yield. Also, as the Master Chemical Mechanism does not have a systematic treatment of epoxides, we divert all epoxide formation to the dicarbonyl product instead. The measurements of SCI and of stabilized CH_2OO indicate[17,18] that most, if not all SCI formed is CH_2OO, owing both to the energy distribution between the fragments, and the lower-energy dissociation channels for MACRO and MVKO. The measured yields of the co-product aldehydes MACR and MVK furthermore indicate that the yield of stabilized CH_2OO is about equal to its total yield, i.e. little decomposition occurs through excited CH_2OO. We remove minor channels from the mechanism by assuming that all CH_2OO formed is stabilized, and that it is the only stabilized SCI formed.

The ozonolysis of MACR and MVK is not treated here, as its contribution is expected to be minor in our experiments; we adopt the mechanism as currently implemented in the MCM v3.3.1.

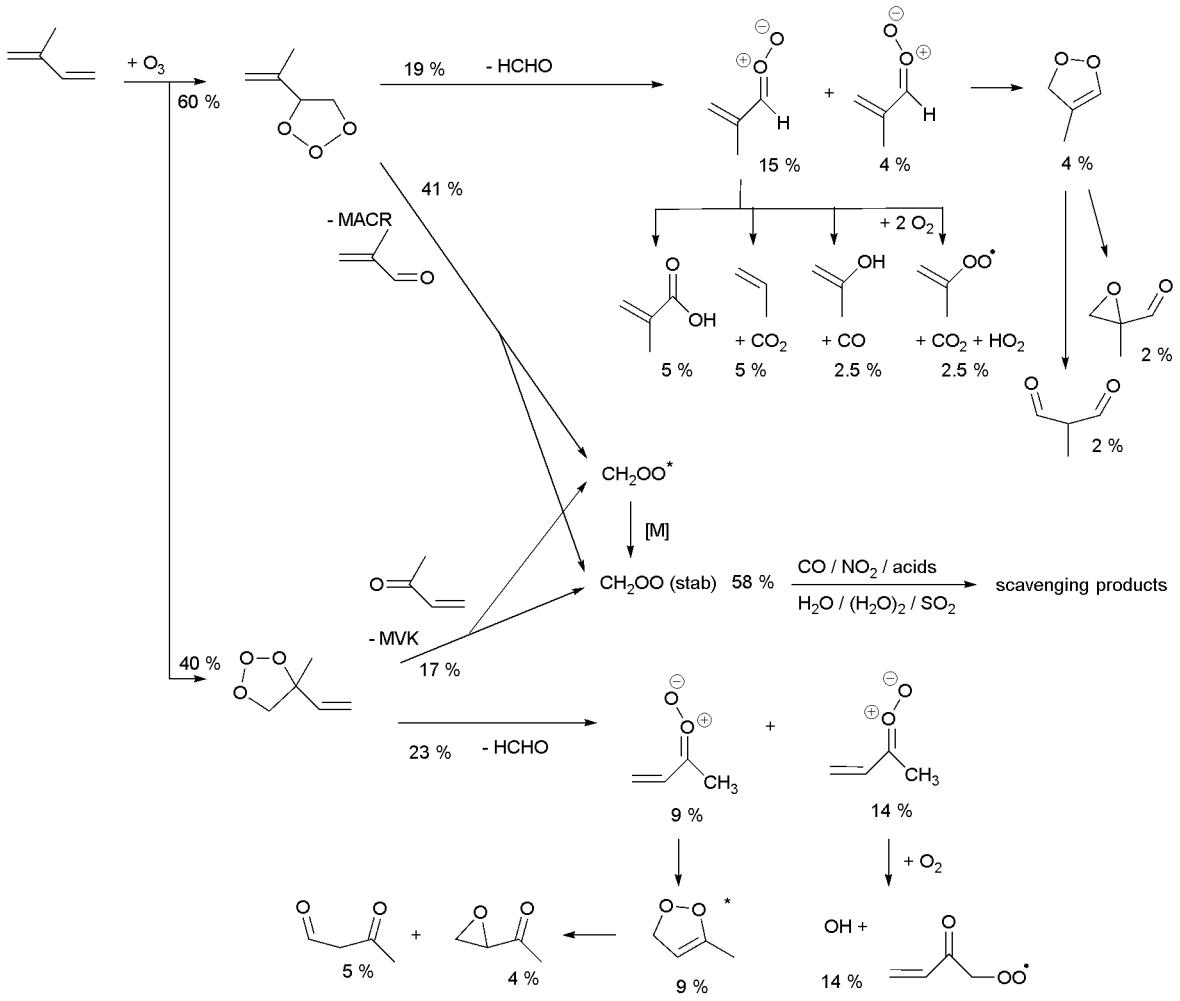

Figure S7: Reaction scheme for the ozonolysis of isoprene

H. RO_2 isomer-specific detectability in the ROxLIF

The RO_2 population in our experiments is dominated by the nascent nitrate-RO_2 from the isoprene + OH + O_2 reaction, with minor contributions of other RO_2 (see Figure S14). The detectability after sampling from the SAPHIR chamber is a function of the amount of OH generated in the fluorescence cell, after partial conversion of the nitrate-RO_2 or epoxy-RO_2 to HO_2 or OH in the converter upstream of the fluorescence cell. To determine the relative conversion efficiency of each RO_2, the chemistry in the converter and fluorescence cell was modelled with their operational conditions during the experiments described in this study. We define the relative conversion efficiency as the ratio between the OH formed from the RO_2 of interest and the OH formed from the reference RO_2 (CH_3OO, used to calibrate the ROxLIF) at the point where its fluorescence is detected.

Table S3: RO_2-specific relative conversion efficiency as a function of temperature

Nitrate-RO_2 isomer	**298 K**	**308 K**	**318 K**
Reference RO_2 ($CH_3OO^{\bullet}$)	1.00	1.00	1.00
1-NO_3-isoprene-2-$OO^{\bullet}$	0.25	0.24	0.21
E-1-NO_3-isoprene-4-$OO^{\bullet}$	0.15	0.16	0.18
Z-1-NO_3-isoprene-4-$OO^{\bullet}$	0.11	0.13	0.14
4-NO_3-isoprene-3-$OO^{\bullet}$	2.7×10^{-2}	2.7×10^{-2}	2.7×10^{-2}
E-4-NO_3-isoprene-1-$OO^{\bullet}$	4.8×10^{-3}	1.9×10^{-3}	8.0×10^{-4}
Z-4-NO_3-isoprene-1-$OO^{\bullet}$	2.0×10^{-5}	1.8×10^{-5}	1.5×10^{-5}
syn-1-NO_3-2,3-epoxy-isoprene-4-$OO^{\bullet}$	3.2×10^{-6}	2.8×10^{-6}	2.6×10^{-6}
anti-1-NO_3-2,3-epoxy-isoprene-4-$OO^{\bullet}$	0.81	0.85	0.87
1-NO_3-2,3-epoxy-4-OH-isoprene-5-$OO^{\bullet}$	0.91	0.94	0.98
1-NO_3-3,4-epoxy-isoprene-2-$OO^{\bullet}$	0.14	0.15	0.18
1-NO_3-4-OH-isoprene-5-$OO^{\bullet}$	0.87	0.89	0.95
4-NO_3-1,2-epoxy-isoprene-3-$OO^{\bullet}$	0.14	0.07	0.04
syn-4-NO_3-2,3-epoxy-isoprene-1-$OO^{\bullet}$	2.7×10^{-4}	2.8×10^{-4}	2.8×10^{-4}
anti-4-NO_3-2,3-epoxy-isoprene-1-$OO^{\bullet}$	0.76	0.78	0.79

The sensitivity of the relative conversion efficiency to various parameters in the model was probed by a brute force error analysis. The relative conversion efficiency was found to be only weakly sensitive to the physical characteristics of the converter (< ±1 % relative for a 15 % change in the estimated residence time), or the fluorescence cell (< ±4 % relative

change for an 18 % change in the estimated residence time), because the absolute conversion efficiency changes similarly for the reference RO_2 ($CH_3OO^{\bullet}$). As shown in Table S3, the relative detectability is also only moderately influenced by temperature (of the order of ±20 % relative change for a 20 K change in temperature). These modelled sensitivities reflect the generally robust operation of the ROxLIF measurement system.

The main uncertainty on the relative conversion efficiency is then due to the uncertainty in the chemistry in the converter and fluorescence cell, where the individual rate coefficients of the many competing reactions determining the overall HO_2 yield at the end of the converter, and the OH yield at the measurement point in the fluorescence cell. To probe this uncertainty, we modified the relative rate for the two epoxidation channels in the 1-NO_3-isoprene-2-$O^{\bullet}$ radical from 2:1 to 1:1, *i.e.* changing the rate coefficient by a factor of 2, which is within the uncertainty of the theoretical predictions. This reduces the predicted relative conversion efficiency for the 1-NO_3-isoprene-2-$OO^{\bullet}$ radical by a factor of 1.55. Lowering the estimated rate of O_2 addition to the 1-NO_3-2,3-epoxy-isoprene-4-yl radicals by a factor of 1.5 reduces the relative conversion efficiency for 1-NO_3-isoprene-2-$OO^{\bullet}$ by 20%. Though not all reaction rates in the degradation schemes are equally critical for the relative conversion efficiency, the reaction schemes for OH/HO_2 formation contain a fairly large number of parameters with an associated uncertainty. We therefore consider the *a priori* estimated relative conversion efficiencies to be only accurate within a factor of 2 to 3. Accounting for this uncertainty, the current model prediction of the detectable RO_2 concentrations in the chamber experiments are in statistical agreement with the measured RO_2 radical signal. Further reducing the uncertainty on the predicted relative conversion efficiencies would require complex explicit experimental calibration for the RO_2 radicals of interest.

I. Chemically activated reactions of 1-NO_3-isoprene-2-O˙ in the converter of the ROxLIF instrument

In the converter, the 1-NO_3-isoprene-2-OO˙ peroxy radical gets converted to 1-NO_3-isoprene-2-O˙ alkoxy radicals by the reaction with NO. We calculate that this reaction is exothermic by 9.47 kcal mol^{-1}. Combined with the thermal energy available in the RO_2 and NO radicals (5-7 kcal mol^{-1} at 298 K), this represents the amount of energy available to the RO + NO_2 products. As explained in detail in earlier work,[19–22] the energy distribution across these products depends on the statistical distribution across the three ensembles of degrees of freedom of the alkoxy radical, the NO_2 radical, and their relative motion, where the large RO moiety tends to receive, on average, the largest part of the distributable energy. The distribution is not fully statistical, due to dynamic effects of the post-transition state dissociation process. On average, though, we can estimate that the alkoxy radical receives a median of about 12 to 15 kcal mol^{-1} of internal energy in a distribution that ranges from zero internal energy to above 20 kcal mol^{-1}.

The energy-specific fate of the alkoxy radical can be estimated by an RRKM master equation analysis as described by Vereecken et al.,[23] which incorporates the energy-specific rate constants for the 1-NO_3-isoprene-2-O˙ radical interconversion to and from the *syn*- and *anti*-1-NO_3-2,3-epoxy-isoprene-4-yl epoxy-alkyl radicals, and the dissociation of the alkoxy radical to MVK + HCHO + NO_2 competing against collisional stabilization; all conformers of each of the intermediates are included in the RRKM calculations. We approximate the collisions in a Troe biexponential energy transfer model, using N_2 as the bath gas (σ = 3.617 Å, ε = 97 K), using σ = 6.0 Å and ε = 350 K for the alkoxy radical, and estimating an average energy transfer per collision of 0.7 kJ mol^{-1}. Thermalization is modelled using a sink starting at 10 kJ mol^{-1} below the dissociation transition state, a limit of internal energy below which it is found that the main fate of the alkoxy radical is thermalization, and where it will react according to the high-pressure rate coefficients derived elsewhere in this work. The probabilities of decomposition as a function of the nascent internal energy are calculated using the DCPD method,[23] and depicted in Figure S8. At 1 atmosphere, we find negligible decomposition across the relevant energy range (not shown). At 25 mbar, as found in the converter, most reactant radicals are stabilized before they decompose, and even at 20 kcal mol^{-1} internal energy, only 5% of the alkoxy radials form MVK + HCHO + NO_2 promptly. As this required energy exceeds the expected internal energy of the alkoxy radical, we conclude that prompt decomposition is not a significant contributor to the fate of the 1-NO_3-isoprene-2-O˙ radicals formed in the 1-NO_3-isoprene-2-O˙ + NO reaction, though a few percent of the alkoxy radicals can still be expected to decompose promptly. The comparatively low contribution of prompt decomposition is due for a large part to the fast interconversion between the alkoxy radical and the near-isoenergetic two epoxy-alkyl radicals, which significantly increases the effective state density for the intermediate compared to the number of reactive states of the dissociation transition state.

Given the expected small contribution, we chose not to perform a more rigorous estimate of the prompt decomposition fraction, and approximate the fate of the 1-NO_3-isoprene-2-OO˙ radical and its products by its thermal reactions, even in the low-pressure converter. Similar considerations apply to the other alkylperoxy radicals in the isoprene-NO_3 reaction system, whose fate we likewise approximate solely as that of the thermalized intermediate.

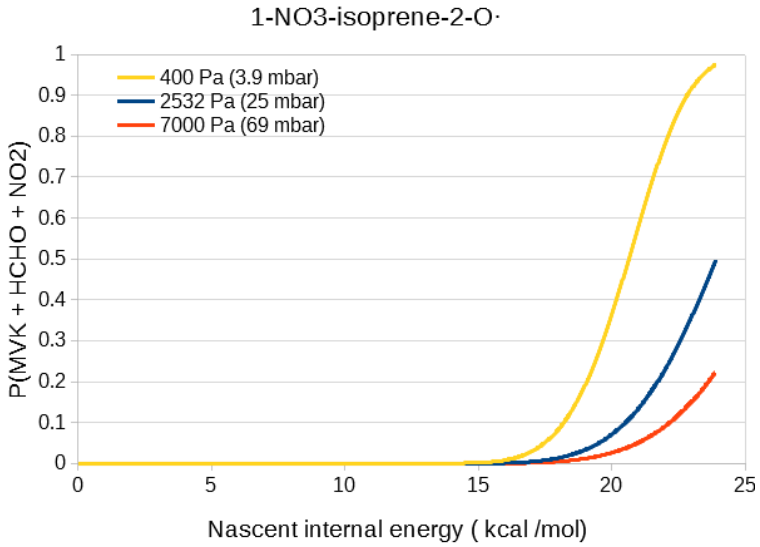

Figure S8: Probability of decomposition of 1-NO_3-isoprene-2-O˙ alkoxy radicals to MVK + HCHO + NO_2 as a function of the nascent internal energy, for various pressures. The remaining fraction is expected to be thermalized, and near-exclusively react as an epoxy-alkyl radical with O_2. For the expected internal energies of the nitrate-RO formed in the nitrate-RO_2 + NO reaction (see text), this suggests a small to negligible contribution of prompt decomposition for the conditions in the converter or the atmosphere.

J. Uncertainties in the HO_2 concentration measured by LIF

Figure S9 shows the time-dependent HO_2 concentrations for the three experiments described within this study as obtained by the LIF instrument, alongside the HO_2 concentration predicted by the three models. As can be seen, the FZJ-NO_3-isoprene and CalTech modelled HO_2 is significantly lower than the measurement, while the HO_2 concentration predicted by MCM v3.3.1 model fortuitously corresponds to the measured magnitude, but presents an irreconcilable time dependence. Elucidating the origin of this discrepancy is not straightforward and beyond the scope of this work, but it is worthwhile to consider its possible sources.

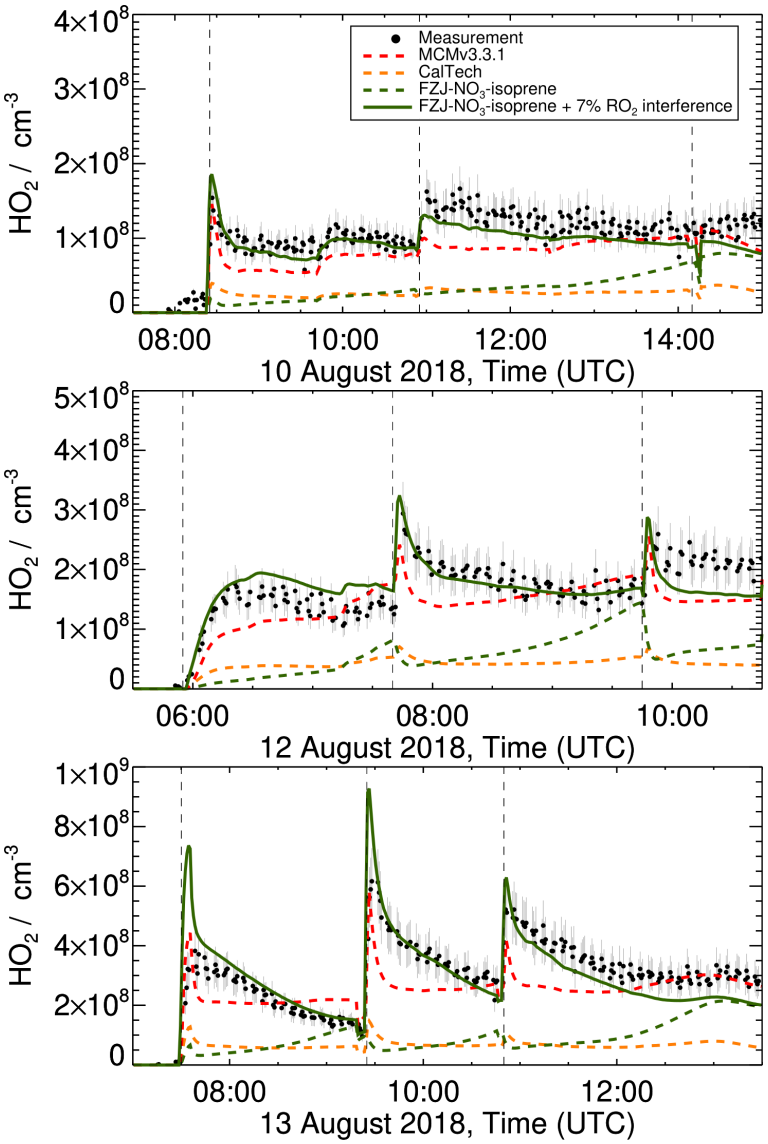

Figure S9: Measured (dots) and modelled (dashed lines, unconstrained) HO_2 concentration. HO_2* (solid line) is derived by assuming an average 7 % interference from all RO_2 in the HO_2 measurement based on the FZJ-NO_3-isoprene model data. A similar analysis using the CalTech model data yields a less favorable agreement for HO_2* due to the lower HO_2 concentration at the end of each injection period, and is not shown.

LIF measurements of HO_2 radicals rely on the conversion of HO_2 radicals to HO in the reaction with NO within the fluorescence cell (~4 hPa). The efficiency of conversion in the specific instrumental setup and experimental conditions is calibrated using a known HO_2 source, allowing the measurement of absolute HO_2 concentrations at the sampling point. However, RO_2 radicals present in the sampled reaction mixture likewise react with NO and can in turn form OH or HO_2 radicals and thus be detected; the total signal consisting of HO_2 contained in the sampled air and additional secondary OH/HO_2 formation from RO_2 is labeled HO_2*. This interference is mitigated by using a low concentration of NO and having a short residence time in the fluorescence cell, which favors the faster HO_2 + NO reaction over slower, multi-step RO_2 + NO reactions. The reduced pressure also suppresses the concentrations of co-reactants, essentially eliminating bimolecular reactions except for reaction with NO and O_2. For typical atmospheric and experimental conditions, this is sufficient to strongly reduce or eliminate RO_2 interference, i.e. $HO_2 \approx HO_2^*$.[24] Due to the reaction conditions in the environmental chamber in the current experiments, RO_2 lifetimes are long and their concentrations are modelled to be up to 10 times higher than HO_2 concentrations, such that even a small yield of HO from RO_2 in the fluorescence cell would lead to a significant interference on the HO_2 measurement. Figure S9 shows the estimated HO_2* obtained by adding an estimated interference signal to the unconstrained modelled HO_2 concentration by assuming that the total modelled RO_2 radicals generate on average 7 % of HO in the fluorescence cell. In this case, values for HO_2* can be obtained that closely match the measurements. Such an interference would also reproduce the temporal behavior of the HO_2 measurement, which is intriguingly similar to the time-dependence of the predicted RO_2. One should consider, however, that not all RO_2 radicals have obvious reaction channels that lead to OH formation for the conditions in the fluorescence cell, specifically when considering the short time between sampling from from the chamber and the fluorescence detection of OH.

In evaluating whether an average RO_2 interference of 7% as mentioned above is realistic, the specific chemistry of the individual RO_2 in the fluorescence cell should then be considered, with particular consideration of the impact of the low pressure, ~ 4 hPa, and the low NO co-reactant concentration in the fluorescence cell.

Potential interference in the HO_2 measurement from RO_2 conversion by 2 reactions with NO

The RO_2 radical reacting with NO forms an alkoxy radical, which can react directly with O_2, forming HO_2, or decompose/isomerise to a substituted alkyl radical which can in turn react with O_2, forming HO_2. Typical examples include the direct, but relatively slow reaction of $CH_3O^{\bullet}$ with O_2 forming HCHO + HO_2, and hydroxylated alkoxy radicals decomposing or isomerising to a >C$^{\bullet}$OH radical, which very rapidly reacts with O_2 forming a carbonyl + HO_2.

The RO_2 radicals in the isoprene+NO_3 reaction mixture can undergo similar reactions, and thus form secondary HO_2 directly in the fluorescence cell, which could be detected after reaction with NO. Compared to atmospheric conditions, the low-pressure environment in the fluorescence cell might even promote HO_2 formation through chemical activation. Indeed, RO_2 + NO → RO + NO_2 reactions are exothermic and the alkoxy radicals formed receive the bulk of the excess energy, leading to energized alkoxy radicals. In atmospheric conditions, this excess is usually dissipated by collisions with the bath gas, but in the low-pressure environment of the fluorescence cell (~ 4 hPa) the excess energy can promote chemical reaction before the excess energy is lost. For example (Figure S3), higher internal energies would increase the yield of HO_2 from 1-NO_3-2-isoprene-4-oxy radicals in the fluorescence cell relative to that found in the atmosphere, by promoting the 1,5-H-shift of the methyl H-atom relative to the energetically more favorable H-shift of the α-ONO_2 H-atom. This HO_2 yield increase in the fluorescence cell is further exacerbated by the lower O_2 concentration, which reduces the competing removal of the 1-

ONO_2-3,4-epoxy-2-yl radical intermediates by recombination with O_2 (estimated thermal pseudo-first order rate coefficient of ~2×10^5 s^{-1}) compared to the atmosphere (k ~ 5×10^7 s^{-1}).

Interference by secondary HO_2 formation in the fluorescence cell is well-known, and mitigation strategies are routinely implemented. Detection of HO_2 in the sampled air requires only a single reaction with NO (HO_2 + NO → OH + NO_2) for conversion to OH, whereas RO_2 leading to HO_2 in the fluorescence cell itself would require two reactions with NO to yield detectable OH (RO_2 + NO → HO_2 + products, followed by HO_2 + NO → OH + NO_2). This type of interference is then counter-acted by the low NO concentrations and short residence times in the fluorescence cell. Furthermore, the NO concentration in the fluorescence cell is modulated by a factor of ~4 to probe this type of interference. For the current experiments, no distinct dependence of the measured HO_2 concentration on the NO concentration was found, suggesting that an interference by conversion of RO_2 to detectable OH by 2 NO reactions cannot explain the large differences between modelled and measured HO_2.

Potential interference in the HO_2 measurement from RO_2 conversion by 1 reaction with NO

RO_2 conversion in the fluorescence cell might also generate OH radicals directly, requiring only a single reaction with NO. This typically requires the presence of a >COOH group, which are known[25,26] to decompose spontaneously to an OH radical when the bearing carbon acquires a free radical due to either H-migration or decomposition (>C˙OOH → >C=O + OH), or eliminate OH in an epoxidation reaction with a β-alkyl radical (>C˙–C(OOH)< → epoxide + OH). Either of these radical intermediates might be formed in the fluorescence cell by decomposition or H-migration reactions of the alkoxy radical formed in the RO_2 + NO reaction. In the current experiments, however, hydroperoxide-substituted RO_2 radicals represent only a small fraction of the peroxy radicals in the chamber (Figure S14), and are thus unlikely to cause interference. Alkyl radicals formed in the fluorescence cell are thus likely to add an O_2 radical, forming a new RO_2 radical.

The addition of O_2 on the intermediate alkyl radicals is, however, highly exothermic by about 25 to 35 kcal mol^{-1}.[27] Under atmospheric pressure, this excess energy is usually lost to the bath gas prior to reaction and the thermal unimolecular reactions of the RO_2 radicals formed are slow, <10 s^{-1},[28] and negligible at the timescales available in the fluorescence cell. In the low-pressure environment of the fluorescence cell, in contrast, collisional energy loss is slow and the energetically hot RO_2 radical formed might undergo unimolecular reactions prior to thermalization. This includes H-migration reactions, which typically have barriers of the order of 20-25 kcal mol^{-1},[28–31] and form a hydroperoxide-substituted alkyl radical which itself might exothermically react with O_2, enabling further chemically activated unimolecular reactions at very short timescales. This includes migration of the α-OOH hydrogen atoms, which is typically rather favorable,[28] and would lead to OH formation as described higher.

The alkoxy radicals formed from the RO_2 radicals generated in the NO_3 + isoprene system are amenable to such reaction sequences. The chemically activated cascade of reactions described above can be initiated from alkyl radicals formed in the fluorescence cell by H-migration reactions in these alkoxy radicals, or by epoxidation reactions in the unsaturated alkoxy radicals leading to alkyl radicals. Furthermore, the initiating alkoxy radical may itself still be chemically activated from the parent RO_2 + NO reaction. An example of this sequence of reactions is illustrated in Figure S10 for the dominant 1-NO_3-isoprene-2-OO˙ peroxy radical (Figure S14). The energized ROOH formed at the end of this sequence might itself be sufficiently highly energized to promptly break the weak peroxide bond (~ 35 kcal mol^{-1}) forming another OH.[32,33]

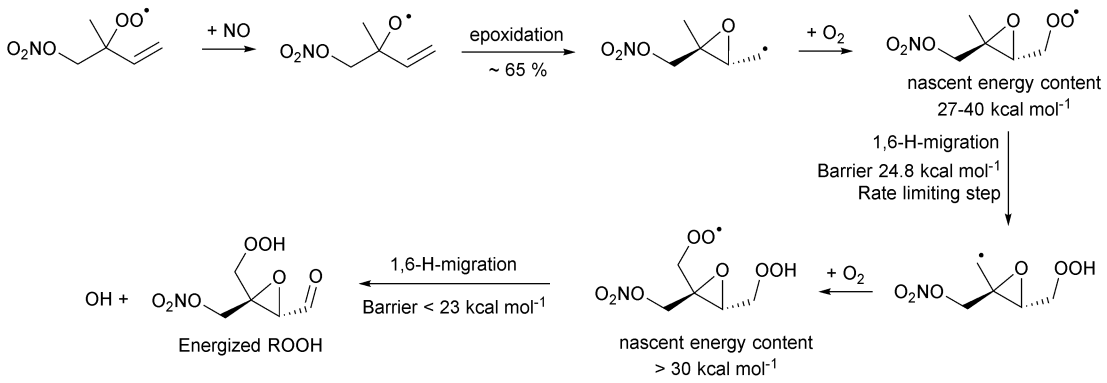

Figure S10: Formation of prompt OH from 1-NO_3-isoprene-2-OO˙ peroxy radical under low-pressure conditions

The above chemistry is highly speculative and is generally not expected to produce high yields of OH. In particular, a (large) fraction of the RO_2 intermediates is still likely to be thermalized, making the necessary H-migrations too slow for the timescales available in the fluorescence cell (< 1 ms). Even for the chemically activated chemistry, there are competing reactions reducing the OH yield. For example, H-migration of the α-ONO_2 hydrogen atoms would yield NO_2 instead of OH. Similarly, hydroxylated RO_2 would likely shift the α-OH hydrogen atoms, generating HO_2 instead of OH and thus require an additional reaction with NO to convert the HO_2 to OH (see above). This sequence is thus unlikely to occur in the RO_2 radicals formed in the OH-initiated oxidation of isoprene, where the initial hydroxy-alkoxy radical formed has a high probability for decomposing or isomerising to an α-OH alkyl radical,[32,33] thus generating HO_2 (see above). In general, then, this type of interference would only be accessible to RO_2 radicals with a substitution pattern suitable for the sequence of reaction needed, with few if any competing reactions.

Despite the low anticipated direct OH yield, only a few percent would be sufficient to cause a significant interference on the HO_2 measurement due to the high relative RO_2 concentrations in the current experiments (Figure S9). Under more atmospheric RO_2:HO_2 ratios closer to 1:1, the interference would be rather small.

In contrast to the above RO_2 to HO_2 conversion which requires 2 reactions with NO to yield detectable OH, the chemically activated reaction sequence yielding OH directly would occur on the same time scale as conversion of sampled HO_2 to OH in the fluorescence cell, and similarly only requires a single reaction with NO. Such an interference in the HO_2 measurements would not be mitigated if the reaction time or NO concentration is reduced and could not be detected by modulation of the NO concentrations during the measurement.

An *a priori* prediction of the OH yields for the RO_2 radicals in the current experiments is highly complex and would be sensitive to parameters such as the molecule-specific collisional thermalization rate, for which neither experimental data nor no reliable theoretical prediction methods exist. Such an estimation is thus outside the scope of the current work.

Potential missing chemistry in the chemical model

The initial chemical steps in the nitrate-initiated oxidation of isoprene were examined in great detail in our theoretical study, and no pathways were discovered that generate a sufficiently high yield of HO_2 to explain the observed HO_2 concentrations. However, it can never be excluded that a pathway was overlooked. It is expected that especially at later times in the experiment where we rely for the oxidation products on chemistry taken from the MCM v3.3.1 and/or CalTech

mechanisms, the chemistry is not adequately described in the current chemical mechanism. Examples for reactions that are not taken into account in those mechanisms concern the large number of intermediates and reactive products, undergoing reactions such as RO_2 H-migrations[28] prevalent in the current reaction conditions, or the specific nitrate-RO chemistry described in this paper and in the study by Novelli et al.[11] Furthermore, the chemistry is also influenced by the OH- and O_3-initiated chemistry of isoprene and any reaction products, and these mechanisms could likewise be missing HO_2 sources that only present themselves under the dark, NO_x-rich reaction conditions of the current experiments and were thus not observable in earlier experiments. A preliminary analysis of an experiment during the NO_3Isop campaign where the oxidation chemistry was dominated by ozone suggested that for these experiments the HO_2 measurements are also significantly higher than the model predictions. It could thus be that the NO_3-initiated chemistry is not the main driver for any missing HO_2 sources in the model.

Concluding remarks

At this time, we do not have sufficient information to unambiguously determine the reasons for the large discrepancy between the modelled and measured HO_2 concentrations. Fur the current work, we thus consider two limiting cases. The first is where we assume that the HO_2 measurement only reflects HO_2 in the sampled air, and that the models are missing some HO_2 sources in any of its branches. This leads to a high-HO_2 concentration scenario that strongly promotes RO_2+HO_2 chemistry. The second limiting case is where the low HO_2 concentrations predicted by the unconstrained model reflects the real HO_2 concentrations in the sampled air, which implies an interference in the HO_2 measurement. This low-HO_2 concentration scenario reduces the importance of RO_2+HO_2 as a loss process for RO_2, promoting unimolecular reactions and RO_2+RO_2 self- and cross-reactions.

K. Experimental concentrations of isoprene and NO_3

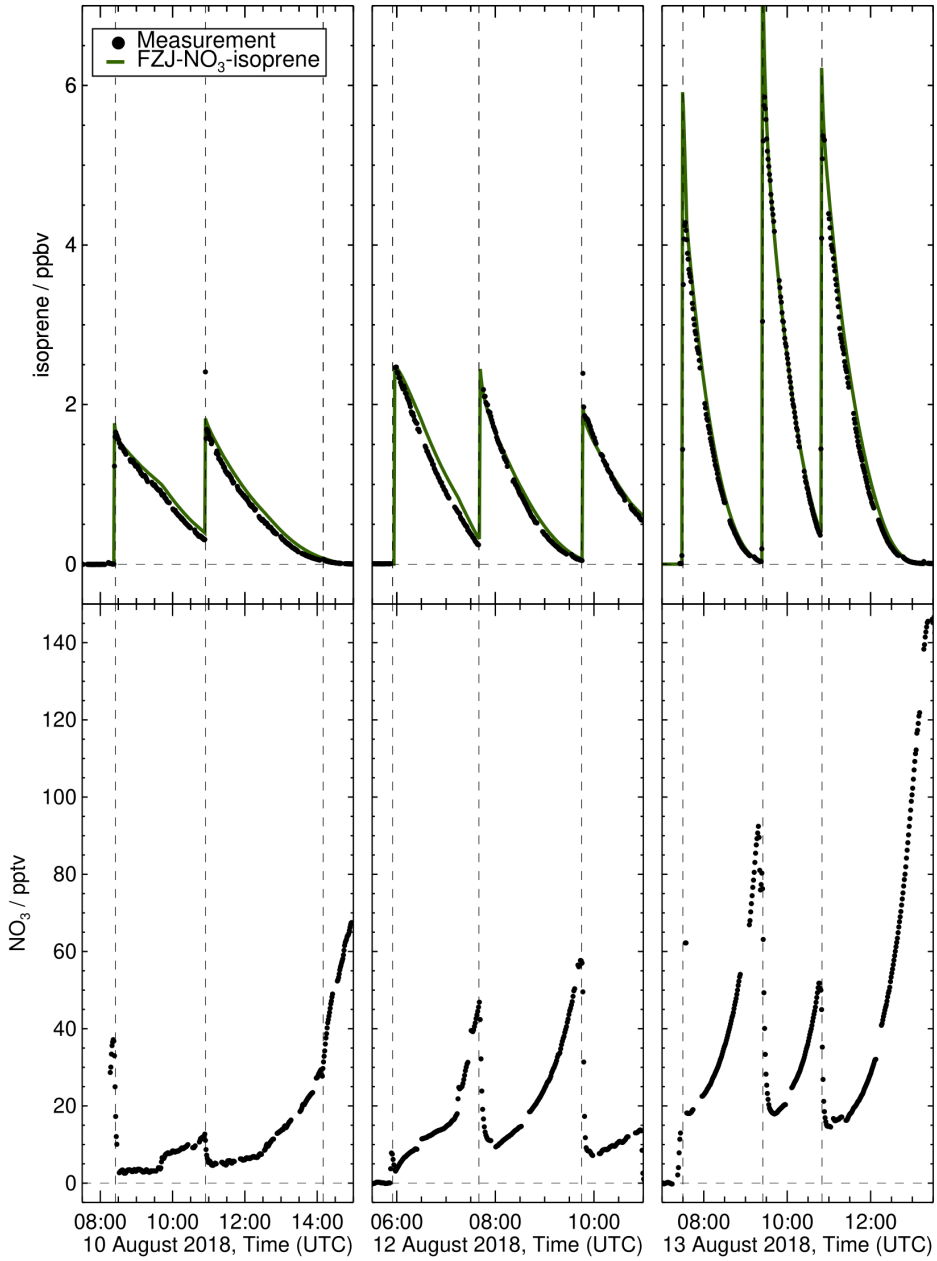

Figure S11: Measured concentration time profiles of isoprene and NO_3 radicals for the three experiments investigated. Also shown is the isoprene concentration time profile as modelled by the FZJ-NO_3-isoprene model.

L. Additional RO_2 concentration time profiles

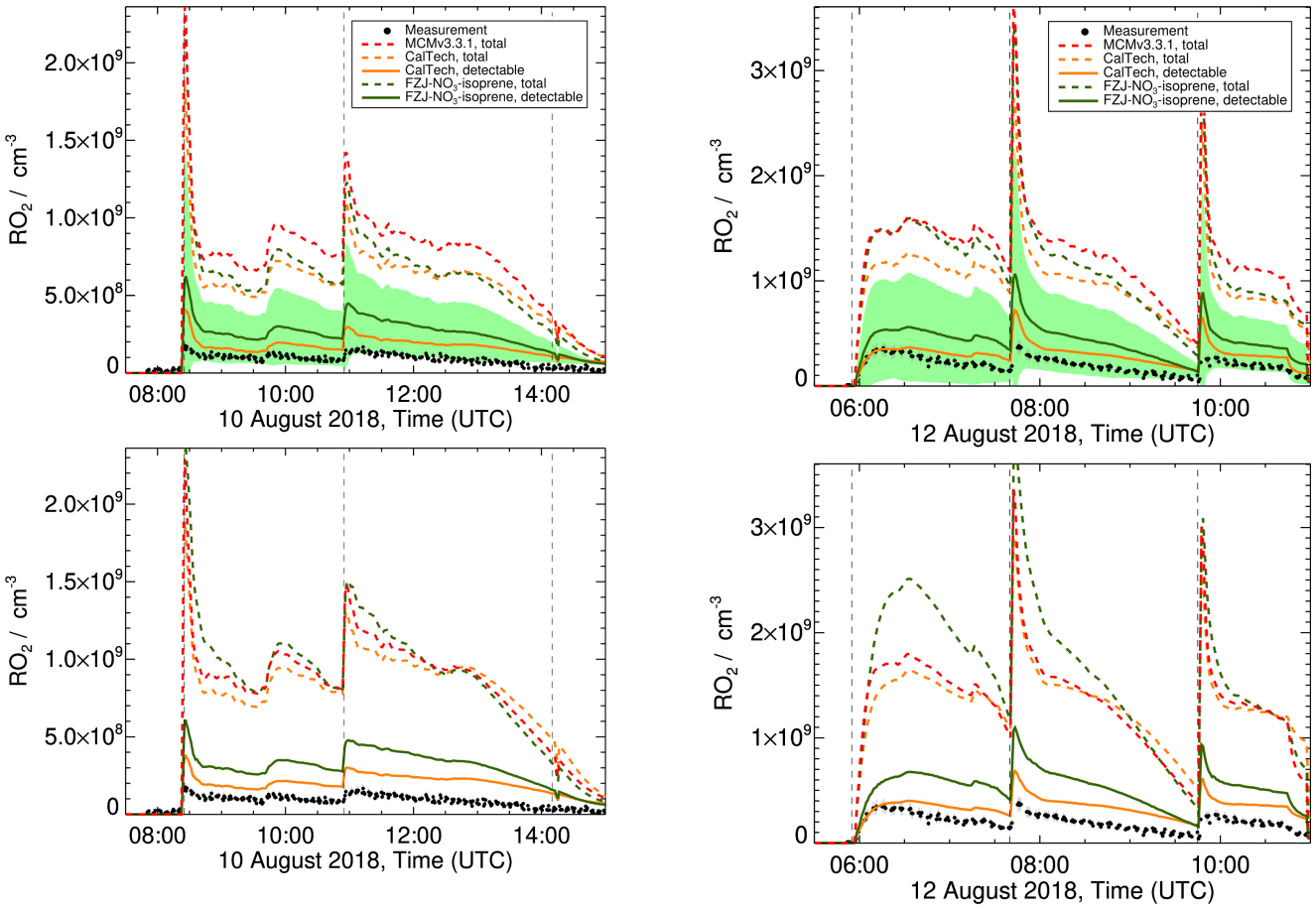

Figure S12: Measured and modelled RO_2 concentration time profiles for the experiments on 10 and 12 Aug 2018. Dashed lines represent the total RO_2 predicted by the models; upper panels: model results with HO_2 constrained to measurements, bottom panels: unconstrained HO_2. For the more detailed CalTech and FZJ-NO_3-isoprene models, additional traces (solid lines) show the estimated detectable RO_2, which can be compared to the measurements. The shaded area shows a factor of 2 uncertainty on the estimated conversion efficiency factors of the detectable RO_2 predicted by the FZJ-NO_3-isoprene model.

M. Additional MVK+MACR concentration time profiles

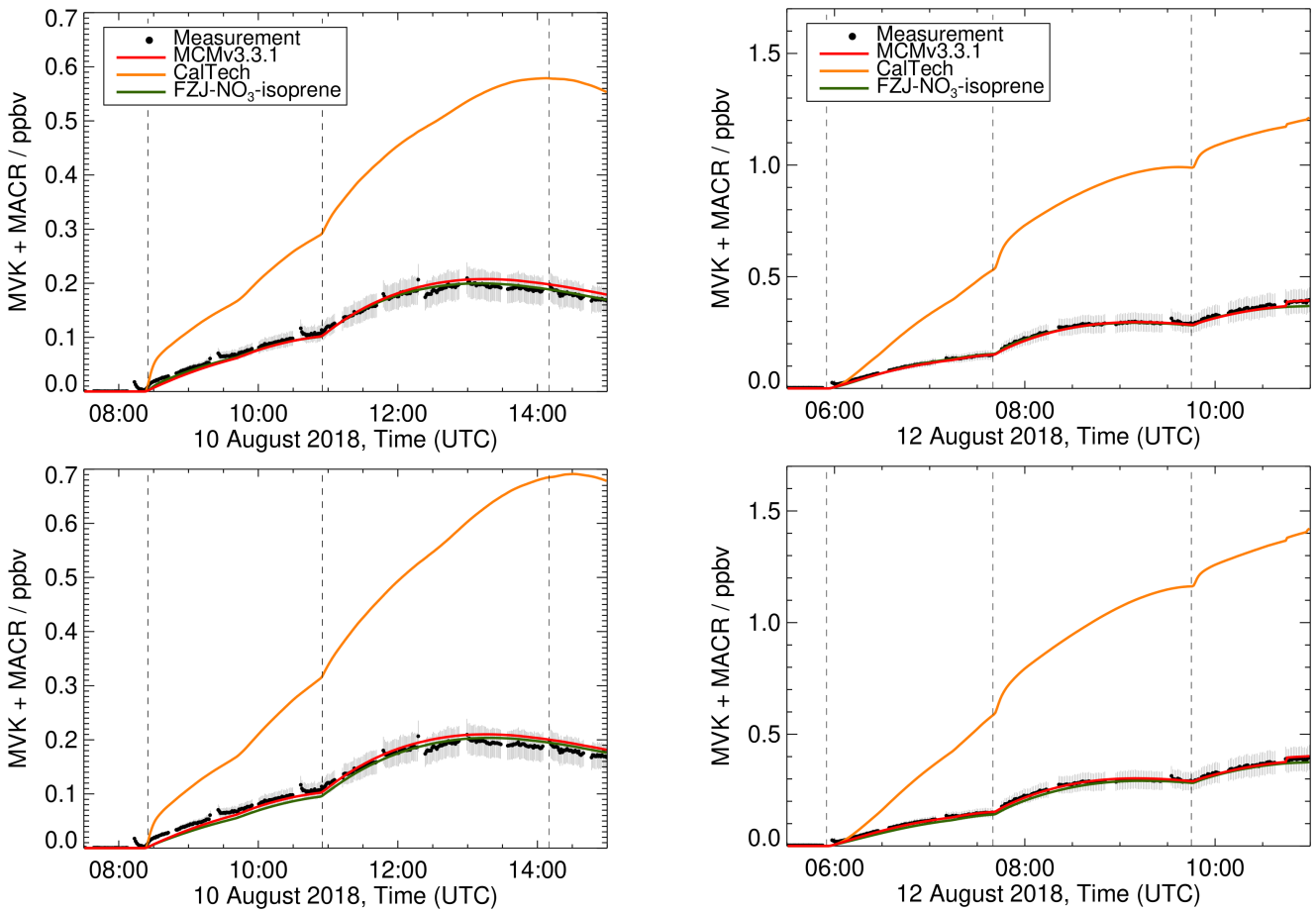

Figure S13: Measured and modelled methyl vinyl ketone + methacrolein (MVK+MACR) concentration time profiles, for the experiments on 10 and 12 Aug 2018; upper panels: model results with HO_2 constrained to measurements, bottom panels: unconstrained HO_2. The measurement assumes equal amounts of MVK and MACR are present to account for the differing sensitivities. For the conditions present in these experiments, this assumption is validated by the modelling.

N. Alkylperoxy radical speciation

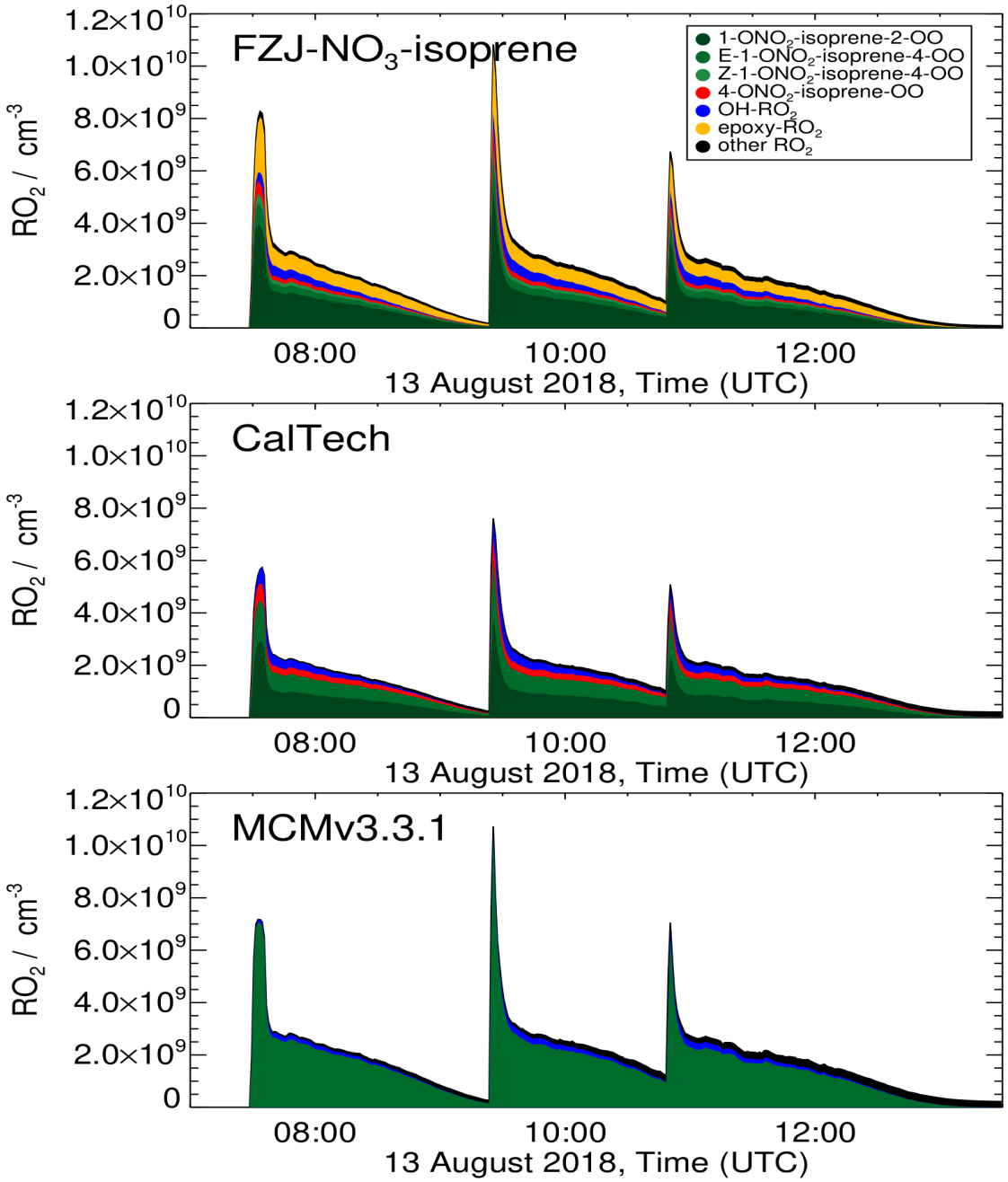

Figure S14: RO_2 speciation in the experiment on 13 Aug 2018, as predicted by the FZJ-NO_3-isoprene (top), CalTech (middle) and MCM v3.3.1 (bottom) models. The main RO_2 radicals from addition of NO_3 on C1 of isoprene are depicted explicitly, while RO_2 radicals with small contributions are lumped into categories, i.e. primary nitrate-RO_2 radicals with the nitrooxy group on carbon C4 (4-ONO_2-isoprene-OO), alkylperoxy radicals originating from the isoprene+OH reaction (OH-RO_2), nitrated epoxy-RO_2 radicals (epoxy-RO_2), and all other RO_2 (including those from ozonolysis). The CalTech and MCM v3.3.1 models do not represent as diverse a set of RO_2 radicals (see main text).

O. Comparison of structure-activity relationships against the direct theoretical calculations

Nitrate peroxy radicals

The results on nitrate-RO_2 presented in the main paper is useful for validating and extending the recent RO_2 H-migration SAR by Vereecken and Nozière;[28] such SAR validation has been put forward by Vereecken et al.[34] to be an important aspect for (semi-)explicit atmospheric mechanism construction. Vereecken and Nozière predicted that H-migration across the trans-substituents in alkenes would have large energy barriers at least up to 1,8-H-migrations and likely beyond. While our current set of calculations does not extend to such large spans, we do find very high barriers exceeding 45 kcal mol^{-1} for 1,5- and 1,6-H-migration between the trans-substituents of the double bond, confirming the SAR predictions for such shorter migration spans. Only two aliphatic 1,4-H-migrations were characterized, and our predictions for these H-migrations are about 3 orders of magnitude above the SAR predictions. These H-migrations are not competitive and the overprediction has no impact here, but it remains useful to trace where the discrepancy originates. In the SAR, the rates for the 1,4-H-migration classes were derived based on lower-level calculations by Miyoshi,[31] and Sharma et al.;[30] it appears that the methodology used in these studies underestimates the rate coefficients by about 3 orders of magnitude. Otkjær et al.[29] and Zhang and Dibble[35] already found similar deviations for some aliphatic 1,4-H-migrations. Combined, this suggests that the SAR[28] for those aliphatic 1,4-H-migrations classes based on the older data[30,31] should be corrected upwards due to methodological shortcomings.

The only aliphatic 1,5-H-migration calculated agrees very well with the SAR predictions, within 10%. For our three 1,5-H-migration with an endo-cyclic double bond forming an allyl-stabilized alkyl radical, the SAR predictions are on average a factor of 3 below our current calculations. Note that the SAR was derived based on *cis*-alkenes whereas we apply it here to *geminal*-substituted alkenes, i.e. where only a single carbon of the double bond is in the TS ring, and the peroxy radical group is not implanted on the double bond. The current result then confirms the generally good transferability of *cis*- to *gem*-alkenes predictions as proposed in the SAR, well within its assumed uncertainty.

For the two fastest H-shifts found in this work, *i.e.* 1,6-shifts of α-ONO_2 allylic H-atoms, the SAR matches our calculations within a factor of 2. For the single 1,6-H-migration of a methyl allylic H-atom, however, the SAR over-predicts the rate by an order of magnitude. The main reason is the $–CH_2ONO_2$ substitution on the double bond, specifically on the central carbon of the product allylic $C^{\bullet}–C=C$ system. For the OH-initiated oxidation of isoprene, a similar large impact by a centrally implanted methyl group in a 1,6-H-migration was observed.[1,36] It thus appears that the RO_2 H-migration SAR should aim to include molecules with more substitutions in the training set to average out their impact. Even then, the SAR for allylic H-migrations will retain a larger intrinsic uncertainty, and more parameters specifying the substitutions around the double bond in allylic H-migrations will need to be added in order to reach SAR prediction accuracy better than a factor of 5.

Nitrate alkoxy radicals

The calculated barrier height for the decomposition reactions listed in the main paper can be compared to those predicted by the SAR by Vereecken and Peeters,[37] with the recent update for β-nitrate alkoxy radicals presented by Novelli et al.[11] The barrier heights for the dominant channels agrees within 1.5 kcal mol^{-1} for all NO_2-forming alkoxy decompositions, and rates are on average within a factor of 10 of the SAR predictions (maximum deviation factor of 76). These deviations are

somewhat larger than typically found for this SAR (see e.g. Novelli et al.[11]), which indicates that multi-substituted alkoxy radicals are susceptible to subtle interactions between the substituents, which are not all accounted for in the SAR.[11,37] For H-migration, we are not aware of a SAR that incorporates the impact of α-ONO_2 substitution or (allylic) migration across double bonds. The SAR by Vereecken and Peeters[33] finds rate coefficients within a factor of 10 at 298 K when substituting an –OH group for the $–ONO_2$ group and ignoring the impact of the double bond; such *ad hoc* substitutions, however, are rather arbitrary and could hide the impact of cancellation of errors. We are not aware of any SAR handling ring closure reactions of alkoxy radicals, but find that the predicted rates for epoxidation are directly comparable to those obtained by Nguyen and Peeters.[38]

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Q. Raw quantum chemical data

The raw quantum chemical data is provided in a separate text file. It contains, for all structures and conformers, the potential energy and geometries at the M06-2X/aug-cc-pVTZ level of theory, as well as the rotational constants, vibrational frequencies, and ZPE corrections. For the lowest conformer(s) of each structure, the potential energy at the CCSD(T)/aug-cc-pVTZ level of theory is also provided, as well as at a few other levels of theory obtained in the course of the CCSD(T) calculations. T1 diagnostics are also provided. The data also shows the relative energy of all the conformers of a particular structure, and their contribution to the Boltzmann equilibrium population at 298 K.

R. The FZJ-NO3-isoprene model in EASY format

```
;#####################################
; FZJ-NO3-ISOPRENE MODEL
;#####################################
; Notational conventions:
; Isoprene-derived radicals and products are labeled on the naming used in the MCM.
; Structures derived from isoprene which are not known in the MCM, or which have a
; more strict meaning here, are named based on a "ISOP" stem, with indication of
; the substituents added/replaced on the individual carbons of the isoprene
; molecule, numbered as shown below:
;        Structure:  CH2=C(CH3)-CH=CH2
;    Carbon number:  1   2 5    3  4
; Substituents are indicated as follows:
;   N : nitrate (-ONO2) substituent
;   O : radical alkoxy oxygen
;   O2 : radical peroxy oxygens
;   CO : numbered carbon is part of a carbonyl (C=O) substituent
;   OH : Hydroxy (-OH) substituent
;   OOH : Hydroperoxide (-OOH) substituent
;   xyO : epoxide functionality spanning carbons x and y
;   xydb : double bond between carbons x and y
;   R : alkyl radical site
;   xOOy : ROOR dimers with organic parts x and y
; Stereochemistry is indicated using the IUPAC stereoindicators E/Z
;
;############
; Preamble : Variables for SAR by Jenkin et al., ACP, 2019
;############
AlkNitrate5=CONST(((2E-22*exp(5)*M)/(1+((2E-22*exp(5)*M)/(0.43*(T/300.)@(-8)))))*0.41@((1+(log10((2E-
22*exp(5)*M)/(0.43*(T/300.)@(-8))))@(2))@(-1)))
AlkNitrate6=CONST(((2E-22*exp(6)*M)/(1+((2E-22*exp(6)*M)/(0.43*(T/300.)@(-8)))))*0.41@((1+(log10((2E-
22*exp(6)*M)/(0.43*(T/300.)@(-8))))@(2))@(-1)))
AlkNitrate9=CONST(((2E-22*exp(9)*M)/(1+((2E-22*exp(9)*M)/(0.43*(T/300.)@(-8)))))*0.41@((1+(log10((2E-
22*exp(9)*M)/(0.43*(T/300.)@(-8))))@(2))@(-1)))
AlkNitrate10=CONST(((2E-22*exp(10)*M)/(1+((2E-22*exp(10)*M)/(0.43*(T/300.)@(-8)))))*0.41@((1+
(log10((2E-22*exp(10)*M)/(0.43*(T/300.)@(-8))))@(2))@(-1)))
AlkNitrate11=CONST(((2E-22*exp(11)*M)/(1+((2E-22*exp(11)*M)/(0.43*(T/300.)@(-8)))))*0.41@((1+
(log10((2E-22*exp(11)*M)/(0.43*(T/300.)@(-8))))@(2))@(-1)))
AlkNitrate12=CONST(((2E-22*exp(12)*M)/(1+((2E-22*exp(12)*M)/(0.43*(T/300.)@(-8)))))*0.41@((1+
(log10((2E-22*exp(12)*M)/(0.43*(T/300.)@(-8))))@(2))@(-1)))

SARRO2HO2_5NOC=CONST(2.8E-13*exp(1300./T)*(1-exp(-0.23*5)))

;############
; Isoprene NO3 and O2 addition, including RO2 re-equilibration by O2 addition/elimination
;############
```

```
k[C5H8 + NO3 --> CNISOPA ] = CONST(2.95E-12*EXP(-450./T)*0.87*0.5)
k[C5H8 + NO3 --> TNISOPA ] = CONST(2.95E-12*EXP(-450./T)*0.87*0.5)
k[C5H8 + NO3 --> CNISOPC ] = CONST(2.95E-12*EXP(-450./T)*0.13*0.7)
k[C5H8 + NO3 --> TNISOPC ] = CONST(2.95E-12*EXP(-450./T)*0.13*0.3)
k[C5H8 + NO3 --> ISOP1OO2N ] = CONST(2.95E-12*EXP(-450./T)*0.0)  ; disabled
k[C5H8 + NO3 --> ISOP3N4OO ] = CONST(2.95E-12*EXP(-450./T)*0.0)  ; disabled

k[TNISOPA + O2 --> EISOP1N4OO] = CONST(2.5E-12*exp(-480./T))
k[TNISOPA + O2 --> ISOP1N2OO] = CONST(3.0E-12)
k[CNISOPA + O2 --> ISOP1N2OO] = CONST(3.0E-12)
k[CNISOPA + O2 --> ZISOP1N4OO] = CONST(3.5E-12)
k[TNISOPC + O2 --> EISOP1OO4N] = CONST(2.5E-12*exp(-480./T))
k[TNISOPC + O2 --> ISOP3OO4N] = CONST(3.5E-12)
k[CNISOPC + O2 --> ISOP3OO4N] = CONST(3.5E-12)
k[CNISOPC + O2 --> ZISOP1OO4N] = CONST(2.0E-12)
k[EISOP1N4OO --> TNISOPA] = CONST(2.40E15*T@(-0.40)*exp(-8707./T))
k[ISOP1N2OO --> TNISOPA] = CONST(4.68E19*T@(-1.48)*exp(-9713./T))
k[ISOP1N2OO --> CNISOPA] = CONST(4.26E20*T@(-1.80)*exp(-10293./T))
k[ZISOP1N4OO --> CNISOPA] = CONST(7.72E23*T@(-2.94)*exp(-9870./T))
k[EISOP1OO4N --> TNISOPC] = CONST(8.05E16*T@(-0.98)*exp(-9987./T))
k[ISOP3OO4N --> TNISOPC] = CONST(5.64E18*T@(-1.41)*exp(-9947./T)
k[ISOP3OO4N --> CNISOPC] = CONST(2.51E19*T@(-1.34)*exp(-10271./T))
k[ZISOP1OO4N --> CNISOPC] = CONST(7.58E22*T@(-2.74)*exp(-10238./T))

;############
; HO2 and RO2 reactions of primary NO3-isoprene-OO radicals
; RO2+RO2 reactions between the primary nitrate-RO2 are included explicitly, while
; reactions with other RO2 are modelled in a lumped way as implemented in the MCM.
;    Variable RO2 : Sum of all RO2 concentrations
;    Variable RRO2 : Sum of all RO2 concentration excluding primary nitrate-RO2
; RO2+HO2 reactions of beta-nitrate-RO2 yield 50% RO+OH, the remainder ROOH
; Reaction rates as in Jenkin et al. ACP, 2019
;############
; HO2 reactions
k[ISOP1N2OO + HO2 -->  ISOP1N2OOH ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[ISOP1N2OO + HO2 -->  OH + ISOP1N2O ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[EISOP1N4OO + HO2 -->  ISOP1N4OOH ] = CONST(2.8E-13*EXP(1300./T)*0.87)
k[ZISOP1N4OO + HO2 -->  ISOP1N4OOH ] = CONST(2.8E-13*EXP(1300./T)*0.87)
k[ISOP3OO4N + HO2 -->  ISOP3OOH4N ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[ISOP3OO4N + HO2 -->  OH + ISOP3O4N ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[EISOP1OO4N + HO2 -->  ISOP1OOH4N ] = CONST(2.8E-13*EXP(1300./T)*0.87)
k[ZISOP1OO4N + HO2 -->  ISOP1OOH4N ] = CONST(2.8E-13*EXP(1300./T)*0.87)
k[ISOP1OO2N + HO2 -->  ISOP1OOH2N ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[ISOP1OO2N + HO2 -->  ISOP1O2N + OH ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[ISOP3N4OO + HO2 -->  ISOP3N4OOH ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)
k[ISOP3N4OO + HO2 -->  ISOP3N4O + OH ] = CONST(2.8E-13*EXP(1300./T)*0.87*0.5)

; RO2 + RO2 reactions between primary nitrate-RO2
```

```
k[EISOP1N4OO + EISOP1N4OO --> EISOP1N4O +  EISOP1N4O ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[EISOP1N4OO + EISOP1N4OO --> ISOP1N4CO + EISOP1N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + EISOP1N4OO --> ISOP1N4CO + ZISOP1N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + EISOP1N4OO --> ISOP1N4OOISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[EISOP1N4OO + ISOP1OO2N --> EISOP1N4O + ISOP1O2N ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[EISOP1N4OO + ISOP1OO2N --> EISOP1N4OH + ISOP1CO2N ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ISOP1OO2N --> ISOP1N4CO + ISOP1OH2N ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ISOP1OO2N --> ISOP1OO2NISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[EISOP1N4OO + ISOP3N4OO --> EISOP1N4O + ISOP3N4O ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[EISOP1N4OO + ISOP3N4OO --> EISOP1N4OH + ISOP3N4CO ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ISOP3N4OO --> ISOP1N4CO + ISOP3N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ISOP3N4OO --> ISOP1N4OOISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[EISOP1N4OO + ZISOP1N4OO --> EISOP1N4O + ZISOP1N4O ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[EISOP1N4OO + ZISOP1N4OO --> EISOP1N4OH + ISOP1N4CO ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ZISOP1N4OO --> ISOP1N4OOISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[EISOP1N4OO + ZISOP1N4OO --> ZISOP1N4OH + ISOP1N4CO ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ZISOP1OO4N --> EISOP1N4O + ZISOP1O4N ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[EISOP1N4OO + ZISOP1OO4N --> EISOP1N4OH + ISOP1CO4N ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ZISOP1OO4N --> ISOP1N4CO + ZISOP1OH4N ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[EISOP1N4OO + ZISOP1OO4N --> ISOP1OO4NISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[EISOP1OO4N + EISOP1N4OO --> EISOP1O4N + EISOP1N4O ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[EISOP1OO4N + EISOP1N4OO --> EISOP1OH4N + ISOP1N4CO ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5*0.5)
k[EISOP1OO4N + EISOP1N4OO --> ISOP1CO4N + EISOP1N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5*0.5)
k[EISOP1OO4N + EISOP1N4OO --> ISOP1CO4N + ZISOP1N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5*0.5)
k[EISOP1OO4N + EISOP1N4OO --> ISOP1OO4NISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[EISOP1OO4N + EISOP1N4OO --> ZISOP1OH4N + ISOP1N4CO ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5*0.5)
k[ISOP1N2OO + EISOP1N4OO --> ISOP1N2O + EISOP1N4O ] = CONST(1.0E-13*EXP(-117/T)*0.8)
k[ISOP1N2OO + EISOP1N4OO --> ISOP1N2OOISOP1N4 ] = CONST(1.0E-13*EXP(-117/T)*0.035)
k[ISOP1N2OO + EISOP1N4OO --> ISOP1N4CO + ISOP1N2OH ] = CONST(1.0E-13*EXP(-117/T)*0.165)
k[ISOP1N2OO + EISOP1OO4N --> ISOP1N2O + EISOP1O4N ] = CONST(1.0E-13*EXP(-117/T)*0.8)
k[ISOP1N2OO + EISOP1OO4N --> ISOP1N2OH + ISOP1CO4N ] = CONST(1.0E-13*EXP(-117/T)*0.165)
k[ISOP1N2OO + EISOP1OO4N --> ISOP1OO4NISOP1N2 ] = CONST(1.0E-13*EXP(-117/T)*0.035)
k[ISOP1N2OO + ISOP1N2OO --> ISOP1N2O + ISOP1N2O ] = CONST(1.0E-13*EXP(-1766/T)*0.965)
k[ISOP1N2OO + ISOP1N2OO --> ISOP1N2OOISOP1N2 ] = CONST(1.0E-13*EXP(-1766/T)*0.035)
k[ISOP1N2OO + ISOP1OO2N --> ISOP1N2O + ISOP1O2N ] = CONST(1.0E-13*EXP(-117/T)*0.8)
k[ISOP1N2OO + ISOP1OO2N --> ISOP1N2OH + ISOP1CO2N ] = CONST(1.0E-13*EXP(-117/T)*0.165)
k[ISOP1N2OO + ISOP1OO2N --> ISOP1OO2NISOP1N2 ] = CONST(1.0E-13*EXP(-117/T)*0.035)
k[ISOP1N2OO + ISOP3N4OO --> ISOP1N2O + ISOP3N4O ] = CONST(1.0E-13*EXP(-117/T)*0.8)
k[ISOP1N2OO + ISOP3N4OO --> ISOP1N2OH + ISOP3N4CO ] = CONST(1.0E-13*EXP(-117/T)*0.165)
k[ISOP1N2OO + ISOP3N4OO --> ISOP3N4OOISOP1N2 ] = CONST(1.0E-13*EXP(-117/T)*0.035)
k[ISOP1N2OO + ISOP3OO4N --> ISOP1N2O + ISOP3O4N ] = CONST(1.0E-13*EXP(-471/T)*0.8)
k[ISOP1N2OO + ISOP3OO4N --> ISOP1N2OH + ISOP3CO4N ] = CONST(1.0E-13*EXP(-471/T)*0.165)
k[ISOP1N2OO + ISOP3OO4N --> ISOP3OO4NISOP1N2 ] = CONST(1.0E-13*EXP(-471/T)*0.035)
k[ISOP1N2OO + ZISOP1N4OO --> ISOP1N2O + ZISOP1N4O ] = CONST(1.0E-13*EXP(-117/T)*0.8)
k[ISOP1N2OO + ZISOP1N4OO --> ISOP1N2OOISOP1N4 ] = CONST(1.0E-13*EXP(-117/T)*0.035)
k[ISOP1N2OO + ZISOP1N4OO --> ISOP1N4CO + ISOP1N2OH ] = CONST(1.0E-13*EXP(-117/T)*0.165)
k[ISOP1N2OO + ZISOP1OO4N --> ISOP1N2O + ZISOP1O4N ] = CONST(1.0E-13*EXP(-117/T)*0.8)
k[ISOP1N2OO + ZISOP1OO4N --> ISOP1N2OH + ISOP1CO4N ] = CONST(1.0E-13*EXP(-117/T)*0.165)
```

```
k[ISOP1N2OO + ZISOP1OO4N --> ISOP1OO4NISOP1N2 ] = CONST(1.0E-13*EXP(-117/T)*0.035)
k[ISOP1OO2N + ISOP1OO2N --> ISOP1O2N + ISOP1O2N ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[ISOP1OO2N + ISOP1OO2N --> ISOP1OH2N + ISOP1CO2N ] = CONST(1.0E-13*EXP(1326/T)*0.365)
k[ISOP1OO2N + ISOP1OO2N --> ISOP1OO2NISOP12N ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[ISOP3N4OO + ISOP3N4OO --> ISOP3N4O + ISOP3N4O ] = CONST(1.0E-13*EXP(1326/T)*0.6)
k[ISOP3N4OO + ISOP3N4OO --> ISOP3N4OH + ISOP3N4CO ] = CONST(1.0E-13*EXP(1326/T)*0.365)
k[ISOP3N4OO + ISOP3N4OO --> ISOP3N4OOISOP3N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[ISOP3OO4N + EISOP1N4OO --> ISOP3CO4N + EISOP1N4OH ] = CONST(1.0E-13*EXP(972/T)*0.365*0.5*0.5)
k[ISOP3OO4N + EISOP1N4OO --> ISOP3CO4N + ZISOP1N4OH ] = CONST(1.0E-13*EXP(972/T)*0.365*0.5*0.5)
k[ISOP3OO4N + EISOP1N4OO --> ISOP3O4N + EISOP1N4O ] = CONST(1.0E-13*EXP(972/T)*0.6)
k[ISOP3OO4N + EISOP1N4OO --> ISOP3OH4N + ISOP1N4CO ] = CONST(1.0E-13*EXP(972/T)*0.365*0.5)
k[ISOP3OO4N + EISOP1N4OO --> ISOP3OO4NISOP1N4 ] = CONST(1.0E-13*EXP(972/T)*0.035)
k[ZISOP1N4OO + ZISOP1N4OO --> ISOP1N4CO + EISOP1N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[ZISOP1N4OO + ZISOP1N4OO --> ISOP1N4CO + ZISOP1N4OH ] = CONST(1.0E-13*EXP(1326/T)*0.365*0.5)
k[ZISOP1N4OO + ZISOP1N4OO --> ISOP1N4OOISOP1N4 ] = CONST(1.0E-13*EXP(1326/T)*0.035)
k[ZISOP1N4OO + ZISOP1N4OO --> ZISOP1N4O +  ZISOP1N4O ] = CONST(1.0E-13*EXP(1326/T)*0.6)

; RO2 + RO2 reactions of primary nitrate-RO2 with other RO2
k[ISOP1N2OO + RRO2 --> ISOP1N2O ] = CONST(1.0E-13*EXP(-490/T)*0.8)
k[ISOP1N2OO + RRO2 --> ISOP1N2OH ] = CONST(1.0E-13*EXP(-490/T)*0.2)
k[EISOP1N4OO + RRO2 --> EISOP1N4O ] = CONST(1.0E-13*EXP(953/T)*0.6)
k[EISOP1N4OO + RRO2 --> ISOP1N4CO ] = CONST(1.0E-13*EXP(953/T)*0.2)
k[EISOP1N4OO + RRO2 --> EISOP1N4OH ] = CONST(1.0E-13*EXP(953/T)*0.2)
k[ZISOP1N4OO + RRO2 --> ZISOP1N4O ] = CONST(1.0E-13*EXP(953/T)*0.6)
k[ZISOP1N4OO + RRO2 --> ZISOP1N4OH ] = CONST(1.0E-13*EXP(953/T)*0.2)
k[ZISOP1N4OO + RRO2 --> ISOP1N4CO ] = CONST(1.0E-13*EXP(953/T)*0.2)
k[ISOP3OO4N + RRO2 --> ISOP3O4N ] = CONST(1.0E-13*EXP(599/T)*0.6)
k[ISOP3OO4N + RRO2 --> ISOP3CO4N ] = CONST(1.0E-13*EXP(599/T)*0.2)
k[ISOP3OO4N + RRO2 --> ISOP3OH4N ] = CONST(1.0E-13*EXP(599/T)*0.2)
k[EISOP1OO4N + RRO2 --> EISOP1O4N ] = CONST(1.0E-13*EXP(953/T)*0.6)
k[EISOP1OO4N + RRO2 --> ISOP1CO4N ] = CONST(1.0E-13*EXP(953/T)*0.2)
k[EISOP1OO4N + RRO2 --> EISOP1OH4N ] = CONST(1.0E-13*EXP(953/T)*0.2)
k[ZISOP1OO4N + RRO2 --> ZISOP1O4N ]  = CONST(1.0E-13*EXP(953/T)*0.6)
k[ZISOP1OO4N + RRO2 --> ISOP1CO4N ]  = CONST(1.0E-13*EXP(953/T)*0.2)
k[ZISOP1OO4N + RRO2 --> ZISOP1OH4N ]  = CONST(1.0E-13*EXP(953/T)*0.2)
k[ZISOP1N4OO + NO3 --> ZISOP1N4O + NO2 ] = CONST(1.9E-11*EXP(-390/T))
k[ZISOP1OO4N + NO3 --> ZISOP1O4N + NO2 ] = CONST(1.9E-11*EXP(-390/T))

;############
; Unimolecular reactions of nitrate-RO2
;############
k[ZISOP1N4OO --> NO2 + C5HPALD1 ]  =  CONST(7.72E-78*T@(28.02)*EXP(4158/T))
k[ZISOP1OO4N --> NO2 + C5HPALD1 ]  =  CONST(2.52E-75*T@(27.06)*EXP(4374/T))
k[ISOP1OO2N --> cyc5ISOP1OO2N ]  =  CONST(8.0)
k[ISOP3N4OO --> cyc5ISOP3N4OO ]  =  CONST(25.0)
k[ISOP1OO2N --> cyc6ISOP1OO2N ]  =  CONST(2.0)
k[ISOP3N4OO --> cyc6ISOP3N4OO ]  =  CONST(1.0)
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;############
; Reaction of primary nitrate-RO2 with NO and NO3
; RO2+NO reaction rate and yields from Jenkin et al., ACP, 2019
; RO2+NO3 reaction rate from Dewald et al., ACP, 2020
;############
k[EISOP1N4OO + NO -->  ISOP1N4N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[EISOP1N4OO + NO --> EISOP1N4O + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[EISOP1OO4N + NO --> EISOP1O4N + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[EISOP1OO4N + NO --> ISOP1N4N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[ISOP1N2OO + NO --> ISOP1N2N ] = CONST(KRO2NO*AlkNitrate9*1.0*0.65)
k[ISOP1N2OO + NO --> ISOP1N2O + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*1.0*0.65))
k[ISOP3OO4N + NO --> ISOP3N4N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[ISOP3OO4N + NO --> ISOP3O4N + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[ZISOP1N4OO + NO -->  ISOP1N4N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[ZISOP1N4OO + NO --> ZISOP1N4O + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[ZISOP1OO4N + NO --> ISOP1N4N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[ZISOP1OO4N + NO --> ZISOP1O4N + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[ISOP1OO2N + NO -->  ISOP1N2N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[ISOP1OO2N + NO --> ISOP1O2N + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[ISOP3N4OO + NO -->  ISOP3N4N ] = CONST(KRO2NO*AlkNitrate9*0.65*1.0)
k[ISOP3N4OO + NO --> ISOP3N4O + NO2 ] = CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[EISOP1N4OO + NO3 --> EISOP1N4O + NO2 ] = CONST(1.9E-11*EXP(-390/T))
k[EISOP1OO4N + NO3 --> EISOP1O4N + NO2 ] = CONST(1.9E-11*EXP(-390/T))
k[ISOP1N2OO + NO3 --> ISOP1N2O + NO2 ] = CONST(1.9E-11*EXP(-390/T))
k[ISOP3OO4N + NO3 --> ISOP3O4N + NO2 ] = CONST(1.9E-11*EXP(-390/T))
k[ISOP1OO2N + NO3 --> ISOP1O2N + NO2 ] = CONST(1.9E-11*EXP(-390/T)) ;(8.9E-12*EXP(-390/T))
k[ISOP3N4OO + NO3 --> ISOP3N4O + NO2 ] = CONST(1.9E-11*EXP(-390/T)) ;(8.9E-12*EXP(-390/T))

;############
; RO2 + HO2 chemistry of gamma- and delta-ONO2-RO2
; This differs from CalTech by not including the RO + OH product channel
;############
k[ISOP1N2OOH3OO4OH + HO2 --> ISOP1N2OOH3OOH4OH ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1N2OOH3OH4OO + HO2 --> ISOP1N2OOH3OH4OOH ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1N2OH3OO4OOH + HO2 --> ISOP1N2OH3OOH4OOH ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1N2OO3OH4OOH + HO2 --> OH + NOA + HCOCH2OOH + HO2 ] = CONST(0.85*2.64E-13*EXP(1300./T))
k[ISOP1N2OO3OH4OOH + HO2 --> ISOP1N2OOH3OH4OOH ] = CONST(0.15*2.64E-13*EXP(1300./T))
k[ISOP1OH2OO3OOH4N + HO2 --> ISOP1OH2OOH3OOH4N ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1OO2OH3OOH4N + HO2 --> ISOP1OOH2OH3OOH4N ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1OOH2OO3OH4N + HO2 --> ISOP1OOH2OOH3OH4N ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1N2OH3OOH4OO + HO2 --> ISOP1N2OH3OOH4OOH ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1OO2OOH3OH4N + HO2 --> ISOP1OOH2OOH3OH4N ] = CONST(2.64E-13*EXP(1300./T))
k[ISOP1N2OH3CO4OO + HO2 --> ISOP1N2OH3CO4OOH ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1N2OH3OO4CO + HO2 --> ISOP1N2OH3OOH4CO ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1OH2OO3CO4N + HO2 --> ISOP1OH2OOH3CO4N ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1CO2OO3OH4N + HO2 --> ISOP1CO2OOH3OH4N ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1N2OH3OO4OH + HO2 --> ISOP1N2OH3OOH4OH ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1OH2OH3OO4N + HO2 --> ISOP1OH2OH3OOH4N ] = CONST(2.6E-13*EXP(1300./T)*0.35)
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k[ISOP1OH2OH3OO4N + HO2 --> OH + HO2 + ACETOL + NO3CH2CHO ] = CONST(2.6E-13*EXP(1300./T)*0.65)
k[ISOP1OH2OO3OH4N + HO2 --> ISOP1OH2OOH3OH4N ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1N2OH3OH4OO + HO2 --> ISOP1N2OH3OH4OOH ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1OO2OH3OH4N + HO2 --> ISOP1OOH2OH3OH4N ] = CONST(2.6E-13*EXP(1300./T))

;############
; Degradation mechanisms of alkoxy radicals
; This includes epoxidation, O2 addition on the epoxyalkyl radicals, and the subsequent
; oxidation mechanisms described in this work.
;############
;ISOP1N2O
k[ISOP1N2O-->NO2+HCHO+MVK]=CONST(2.69E6*T@(2.24)*EXP(-4491/T))
k[ISOP1N2O-->CH3O2+NMVK]=CONST(1.00E6*T@(2.47)*EXP(-6325/T))
k[ISOP1N2O-->ZISOP1N23O4R]=CONST(8.96E9*T@(0.78)*EXP(-2207/T))
k[ISOP1N2O-->EISOP1N23O4R]=CONST(4.24E9*T@(0.92)*EXP(-1996/T))
k[ZISOP1N23O4R-->ISOP1N2O]=CONST(7.42E9*T@(0.95)*EXP(-2535/T))
k[EISOP1N23O4R-->ISOP1N2O]=CONST(1.57E10*T@(0.80)*EXP(-2489/T))
k[ZISOP1N23O4R + O2 -->ZISOP1N23O4OO] = CONST(7.5E-12)
k[EISOP1N23O4R + O2 -->EISOP1N23O4OO] = CONST(7.5E-12)
k[ZISOP1N23O4OO --> ISOP1CO23O4OOH + NO2] = CONST(3.6E-5)
k[ZISOP1N23O4OO + RO2 --> ZISOP1N23O4O] = CONST(1.0E-13*EXP(1139/T)*0.2)
k[ZISOP1N23O4OO + RO2 --> ISOP1N23O4CO] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[ZISOP1N23O4OO + RO2 --> ISOP1N23O4OH] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[ZISOP1N23O4OO + NO3 --> ZISOP1N23O4O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[ZISOP1N23O4OO + HO2 --> ISOP1N23O4OOH] = CONST(2.8E-13*EXP(1300./T)*0.9)
k[ZISOP1N23O4OO + NO --> ZISOP1N23O4O + NO2]=CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[ZISOP1N23O4OO + NO --> ZISOP1N23O4N]=CONST(KRO2NO*(1-AlkNitrate9*0.65*1.0))
k[EISOP1N23O4OO --> ISOP1N23O4CO5OOH + OH]=CONST(4.1E-6)
k[EISOP1N23O4OO + RO2 --> EISOP1N23O4O] = CONST(1.0E-13*EXP(1139/T)*0.2)
k[EISOP1N23O4OO + RO2 --> ISOP1N23O4CO] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[EISOP1N23O4OO + RO2 --> ISOP1N23O4OH] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[EISOP1N23O4OO + NO3 --> EISOP1N23O4O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[EISOP1N23O4OO + HO2 --> ISOP1N23O4OOH] = CONST(2.8E-13*EXP(1300./T)*0.9)
k[EISOP1N23O4OO + NO --> EISOP1N23O4O + NO2]=CONST(KRO2NO*(1-AlkNitrate10*0.65*1.0))
k[EISOP1N23O4OO + NO --> EISOP1N23O4N]=CONST(KRO2NO*AlkNitrate10*0.65*1.0)
k[ZISOP1N23O4O + O2 --> HO2 + ISOP1N23O4CO] = CONST(2.5E-14*EXP(-300./T))
k[ZISOP1N23O4O --> IEB1CHO + NO2] = CONST(4.14E-16*T@(8.68)*EXP(477/T))
k[ISOP1N23O4OH + OH --> HO2 + ISOP1N23O4CO] = CONST(3.5E-11*0.5)
k[ISOP1N23O4OH + OH --> NO2 + IEB1CHO] = CONST(3.5E-11*0.5)
k[ISOP1N23O4OH + hv --> NO2 + IEB1CHO] = CONST(J56*4)
k[EISOP1N23O4O + O2 --> HO2 + ISOP1N23O4CO] = CONST(2.5E-14*EXP(-300./T))
k[EISOP1N23O4O --> EISOP1N23O4OH5R] = CONST(3.23E-23*T@(10.99)*EXP(400/T))
k[EISOP1N23O4OH5R --> ISOP1N25db3O4OH] = CONST(1.66E8*T@(1.33)*EXP(-1652/T))
k[ISOP1N25db3O4OH --> EISOP1N23O4OH5R] = CONST(5.74E13*T@(-0.49)*EXP(-3440/T))
k[ISOP1N25db3O4OH --> ZISOP1N23O4OH5R] = CONST(2.09E16*T@(-1.40)*EXP(-4227/T))
k[ZISOP1N23O4OH5R --> ISOP1N25db3O4OH] = CONST(4.04E11*T@(0.24)*EXP(-2337/T))
k[EISOP1N23O4OH5R + O2 --> EISOP1N23O4OH5OO ] = CONST(7.5E-12)
k[ZISOP1N23O4OH5R + O2 --> ZISOP1N23O4OH5OO ] = CONST(7.5E-12)
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k[ISOP1N25db3O4OH --> MACRN4 + HCHO + HO2 ] = CONST(1.39E6*(T)@(2.11)*EXP(-1314/T))
k[ISOP1N25db3O4OH + O2 -->  MACR3N + HCHO + HO2 ] = CONST(2.5E-14*EXP(-300./T))
; The chemistry after E/Z-ISOP1N23O4OH5OO is minor, so drop stereospecificity on products
k[EISOP1N23O4OH5OO --> ISOP1N23O4CO5OOH + HO2 ] = CONST(8.05E-2*T@(3.81)*EXP(-7134/T))
k[EISOP1N23O4OH5OO + RO2 --> EISOP1N23O4OH5O] = CONST(1.0E-13*EXP(1140/T)*0.2)
k[ZISOP1N23O4OH5OO + RO2 --> ZISOP1N23O4OH5O] = CONST(1.0E-13*EXP(1140/T)*0.2)
k[EISOP1N23O4OH5OO + RO2 --> ISOP1N23O4OH5CO] = CONST(1.0E-13*EXP(1140/T)*0.4)
k[ZISOP1N23O4OH5OO + RO2 --> ISOP1N23O4OH5CO] = CONST(1.0E-13*EXP(1140/T)*0.4)
k[EISOP1N23O4OH5OO + RO2 --> ISOP1N23O4OH5OH] = CONST(1.0E-13*EXP(1140/T)*0.4)
k[ZISOP1N23O4OH5OO + RO2 --> ISOP1N23O4OH5OH] = CONST(1.0E-13*EXP(1140/T)*0.4)
k[EISOP1N23O4OH5OO + NO3 --> EISOP1N23O4OH5O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[ZISOP1N23O4OH5OO + NO3 --> ZISOP1N23O4OH5O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[EISOP1N23O4OH5OO + HO2 --> ISOP1N23O4OH5OOH] = CONST(2.8E-13*EXP(1300./T)*0.92*0.5)
k[ZISOP1N23O4OH5OO + HO2 --> ISOP1N23O4OH5OOH] = CONST(2.8E-13*EXP(1300./T)*0.92*0.5)
k[EISOP1N23O4OH5OO + NO --> EISOP1N23O4OH5O + NO2]=CONST(KRO2NO*(1-AlkNitrate11*0.65*0.8))
k[ZISOP1N23O4OH5OO + NO --> ZISOP1N23O4OH5O + NO2]=CONST(KRO2NO*(1-AlkNitrate11*0.65*0.8))
k[EISOP1N23O4OH5OO + NO --> ISOP1N23O4OH5N]=CONST(KRO2NO*AlkNitrate11*0.65*0.8)
k[ZISOP1N23O4OH5OO + NO --> ISOP1N23O4OH5N]=CONST(KRO2NO*AlkNitrate11*0.65*0.8)
k[EISOP1N23O4OH5O + O2 --> ISOP1N23O4CO5OH + HO2] = CONST(2.4E7)                ; 1,5-H-shift
k[ZISOP1N23O4OH5O + O2 --> ISOP1N23O4OH5CO + HO2] = CONST(2.5E-14*EXP(-300./T)) ; direct O2 reaction

;EISOP1N4O
k[ZISOP1N4O --> HC4CCHO + NO2 ] = CONST(8.93E-30*T@(13.31)*EXP(2629/T))
k[ZISOP1N4O + O2 --> ISOP1N4CO + HO2 ] = CONST(2.5E-14*EXP(-300./T))
k[ZISOP1N4O --> ISOP1N2R34O ] = CONST(1.62E12*T@(-0.01)*EXP(-2622/T))
k[EISOP1N4O --> ISOP1N4OH5OO ] = CONST(2.08E-37*T@(15.82)*EXP(2675/T))
k[EISOP1N4O + O2 --> ISOP1N4CO + HO2 ] = CONST(2.5E-14*EXP(-300./T))
k[EISOP1N4O --> ISOP1N2R34O ] = CONST(1.24E10*T@(0.77)*EXP(-2682/T))
k[ISOP1N2R34O --> ZISOP1N4O] = CONST(7.51E8*T@(1.10)*EXP(-2556/T))
k[ISOP1N2R34O --> EISOP1N4O] = CONST(3.86E10*T@(0.72)*EXP(-2887/T))
k[ISOP1N2R34O + O2 --> ISOP1N2OO34O] = CONST(7.5E-12)
k[ISOP1N2OO34O --> ISOP1N2OOH34O4R] = CONST(4.5E-4)
k[ISOP1N2OO34O + RO2 --> ISOP1N2O34O] = CONST(1.0E-13*EXP(118/T)*0.35)
k[ISOP1N2OO34O + RO2 --> ISOP1N23O4OH] = CONST(1.0E-13*EXP(118/T)*0.65)
k[ISOP1N2OO34O + NO3 --> ISOP1N2O34O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[ISOP1N2OO34O + HO2 --> ISOP1N2OOH34O] = CONST(2.8E-13*EXP(1300./T)*0.9*0.5)
k[ISOP1N2OO34O + HO2 --> ISOP1N2O34O + OH] = CONST(2.8E-13*EXP(1300./T)*0.9*0.5)
k[ISOP1N2OO34O + NO --> ISOP1N2O34O + NO2] = CONST(KRO2NO*(1-AlkNitrate10*1.0*0.65))
k[ISOP1N2OO34O + NO --> ISOP1N2N34O] = CONST(KRO2NO*AlkNitrate10*1.0*0.65)
k[ISOP1N2O34O --> NO2 + HCHO + BUT12O3CO] = CONST(2.38E6*T@(2.06)*EXP(-4896/T))
k[ISOP1N2O34O --> ETHOXO2 + NOA] = CONST(7.14E8*T@(1.52)*EXP(-6175/T))
k[ISOP1N4OH5OO --> ISOP1N4CO5OOH + HO2] = CONST(8.05E-02*T@(3.81)*EXP(-7134/T))
k[ISOP1N4OH5OO + RO2 --> ISOP1N4OH5O] = CONST(1.0E-13*EXP(1139/T)*0.2)
k[ISOP1N4OH5OO + RO2 --> ISOP1N4OH5CO] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[ISOP1N4OH5OO + RO2 --> ISOP1N4OH5OH] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[ISOP1N4OH5OO + NO3 --> ISOP1N4OH5O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[ISOP1N4OH5OO + HO2 --> ISOP1N4OH5OOH] = CONST(2.8E-13*EXP(1300./T)*0.9)
k[ISOP1N4OH5OO + NO --> ISOP1N4OH5O + NO2] = CONST(KRO2NO*(1-AlkNitrate11*0.65*1.0))
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k[ISOP1N4OH5OO + NO --> ISOP1N4OH5N] = CONST(KRO2NO*AlkNitrate11*0.65*1.0)
k[ISOP1N4OH5O + O2 --> ISOP1N4OH5CO + HO2] = CONST(2.5E-14*EXP(-300./T))
k[ISOP1N4OH5O --> ISOP1N4CO5OH + HO2] = CONST(2.4E7)

;EISOP1O4N
k[ZISOP1O4N --> HC4ACHO + NO2 ] = CONST(1.35E-27*T@(12.67)*EXP(1997/T))
k[ZISOP1O4N --> ISOP12O3R4N ] = CONST(1.15E9*T@(1.12)*EXP(-2906/T))
k[ZISOP1O4N + O2 --> ISOP1CO4N + HO2 ] = CONST(2.5E-14*EXP(-300./T))
k[EISOP1O4N --> ISOP12O3R4N ] = CONST(8.91E8*T@(1.09)*EXP(-3233/T))
k[EISOP1O4N + O2 --> ISOP1CO4N + HO2 ] = CONST(2.5E-14*EXP(-300./T))
k[ISOP12O3R4N --> ZISOP1O4N] = CONST(3.46E10*T@(0.77)*EXP(-3270/T))
k[ISOP12O3R4N --> EISOP1O4N] = CONST(9.63E11*T@(0.37)*EXP(-3745/T))
k[ISOP12O3R4N + O2 --> ISOP12O3OO4N] = CONST(7.5E-12)
k[ISOP12O3OO4N --> ISOP1R12O3OOH4N] = CONST(1.2E-3) ; Chemistry not considered further
k[ISOP12O3OO4N + RO2 --> ISOP12O3O4N] = CONST(1.0E-13*EXP(891/T)*0.2)
k[ISOP12O3OO4N + RO2 --> ISOP12O3CO4N] = CONST(1.0E-13*EXP(891/T)*0.4)
k[ISOP12O3OO4N + RO2 --> ISOP12O3OH4N] = CONST(1.0E-13*EXP(891/T)*0.4)
k[ISOP12O3OO4N + NO3 --> ISOP12O3O4N + NO2] = CONST(1.9E-11*EXP(-390/T))
k[ISOP12O3OO4N + HO2 --> ISOP12O3OOH4N] = CONST(2.8E-13*EXP(1300./T)*0.9*0.5)
k[ISOP12O3OO4N + HO2 --> ISOP12O3O4N + OH] = CONST(2.8E-13*EXP(1300./T)*0.9*0.5)
k[ISOP12O3OO4N + NO --> ISOP12O3O4N + NO2]=CONST(KRO2NO*(1-AlkNitrate10*1.0*0.65))
k[ISOP12O3OO4N + NO --> ISOP12O3N4N]=CONST(KRO2NO*AlkNitrate10*1.0*0.65)
k[ISOP12O3O4N --> NO2 + HCHO + IBUT12O3CO] = CONST(1.8E13*(T/298)@(1.7)*EXP(-6542/T))
k[ISOP12O3O4N --> CHOCONO2 + EPOXY2PROPYLO2] = CONST(1.8E13*(T/298)@(1.7)*EXP(-6055/T))
k[ISOP12O3O4N + O2 --> HO2 + ISOP12O3CO4N] = CONST(2.5E-14*EXP(-300./T))

;ISOP3O4N
k[ISOP3O4N --> NO2 + HCHO + MACR] = CONST(8.06E5*T@(2.19)*EXP(-3981/T))
k[ISOP3O4N + O2 --> ISOP3CO4N + HO2] = CONST(2.5E-14*EXP(-300./T))
k[ISOP3O4N --> ZISOP1R23O4N] = CONST(1.19E12*T@(0.06)*EXP(-2795/T))
k[ISOP3O4N --> EISOP1R23O4N] = CONST(2.31E10*T@(0.54)*EXP(-2736/T))
k[ZISOP1R23O4N --> ISOP3O4N] = CONST(8.15E10*T@(0.65)*EXP(-2475/T))
k[EISOP1R23O4N --> ISOP3O4N] = CONST(5.53E9*T@(0.93)*EXP(-2142/T))
k[ZISOP1R23O4N + O2 --> ZISOP1OO23O4N] = CONST(7.5E-12)
k[EISOP1R23O4N + O2 --> EISOP1OO23O4N] = CONST(7.5E-12)
k[ZISOP1OO23O4N --> ISOP1OOH23O4CO + NO2] = CONST(1.68E-12*T@(7.19)*EXP(-7173/T))
k[ZISOP1OO23O4N + RO2 --> ZISOP1O23O4N] = CONST(1.0E-13*EXP(1139/T)*0.2)
k[ZISOP1OO23O4N + RO2 --> ISOP1CO23O4N] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[ZISOP1OO23O4N + RO2 --> ISOP1OH23O4N] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[ZISOP1OO23O4N + NO3 --> ZISOP1O23O4N + NO2] = CONST(1.9E-11*EXP(-390/T))
k[ZISOP1OO23O4N + HO2 --> ISOP1OOH23O4N] = CONST(2.8E-13*EXP(1300./T)*0.9)
k[ZISOP1OO23O4N + NO --> ZISOP1O23O4N + NO2]=CONST(KRO2NO*(1-AlkNitrate10*0.65*1.0))
k[ZISOP1OO23O4N + NO --> ISOP1N23O4N]=CONST(KRO2NO*AlkNitrate10*0.65*1.0)
k[ZISOP1O23O4N --> ZISOP1OH23O4CO + NO2] = CONST(3.3E6)
k[ZISOP1O23O4N + O2 --> ZISOP1CO23O4N + HO2] = CONST(2.5E-14*EXP(-300./T))
k[EISOP1OO23O4N + RO2 --> EISOP1O23O4N] = CONST(1.0E-13*EXP(1139/T)*0.2)
k[EISOP1OO23O4N + RO2 --> ISOP1CO23O4N] = CONST(1.0E-13*EXP(1139/T)*0.4)
k[EISOP1OO23O4N + RO2 --> ISOP1OH23O4N] = CONST(1.0E-13*EXP(1139/T)*0.4)
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```
k[EISOP1OO23O4N + NO3 --> EISOP1O23O4N + NO2] = CONST(1.9E-11*EXP(-390/T))
k[EISOP1OO23O4N + HO2 --> ISOP1OOH23O4N] = CONST(2.8E-13*EXP(1300./T)*0.9)
k[EISOP1OO23O4N + NO --> EISOP1O23O4N + NO2]=CONST(KRO2NO*(1-AlkNitrate10*0.65*1.0))
k[EISOP1OO23O4N + NO --> ISOP1N23O4N]=CONST(KRO2NO*AlkNitrate10*0.65*1.0)
k[EISOP1O23O4N + O2 --> ISOP1CO23O4N + HO2] = CONST(2.5E-14*EXP(-300./T))

;ISOP1O2N
k[ISOP1O2N--> NO2 + HCHO + MVK]=CONST(2.69E6*T@(2.24)*EXP(-4491/T))

;ISOP3N4O
k[ISOP3N4O --> NO2 + HCHO + MACR] = CONST(8.06E5*T@(2.19)*EXP(-3981/T))

;############
; Chemistry of epoxyethylperoxy and epoxypropylperoxy
; based on chemistry included in MCM v3.3.1
;############
; Epoxyethylperoxy chemistry from MCM
k[ETHOXO2+HO2-->ETHOXOOH]=CONST(KRO2HO2*0.387)
k[ETHOXO2+NO-->CHOOCH2O2+NO2]=CONST(KRO2NO)
k[ETHOXO2+NO3-->CHOOCH2O2+NO2]=CONST(KRO2NO3)
k[ETHOXO2-->CHOOCH2O2]=CONST(8.8D-13*RO2)
k[ETHOXOOH+OH-->ETHOXO2]=CONST(7.15D-12)
k[ETHOXOOH+hv-->CHOOCH2O2+OH]=CONST(J41)
k[CHOOCH2O2+HO2-->CHOOCH2OOH]=CONST(KRO2HO2*0.387)
k[CHOOCH2O2+NO-->CHOOCH2NO3]=CONST(KRO2NO*0.009)
k[CHOOCH2O2+NO-->NO2+CHOOCH2O]=CONST(KRO2NO*0.991)
k[CHOOCH2O2+NO3-->CHOOCH2O+NO2]=CONST(KRO2NO3)
k[CHOOCH2O2-->CHOOCH2O]=CONST(2.00D-12*0.6*RO2)
k[CHOOCH2O2-->CHOOCH2OH]=CONST(2.00D-12*0.2*RO2)
k[CHOOCH2O2-->CHOOCHO]=CONST(2.00D-12*0.2*RO2)
k[CHOOCH2OOH+OH-->CHOOCH2O2]=CONST(1.90D-12*EXP(190/(T)))
k[CHOOCH2OOH+OH-->CHOOCHO+OH]=CONST(1.63D-11)
k[CHOOCH2OOH+hv-->CHOOCH2O+OH]=CONST(J41)
k[CHOOCH2NO3+OH-->CHOOCHO+NO2]=CONST(2.26D-13)
k[CHOOCH2NO3+hv-->CHOOCH2O+NO2]=CONST(J53)
k[CHOOCH2O-->CHOOCHO+HO2]=CONST(KROPRIM*O2)
k[CHOOCH2O-->HCOOH+HO2+CO]=CONST(2.00D+14*EXP(-6850/(T)))
k[CHOOCH2OH+OH-->CHOOCHO+HO2]=CONST(4.31D-12)

; Epoxy-2-propylperoxy chemistry
k[EPOXY2PROPO2 + NO --> EPOXY2PROPO + NO2]=CONST(KRO2NO*(1-AlkNitrate6*1.0*1.0))
k[EPOXY2PROPO2 + NO --> EPOXY2PROPONO2]=CONST(KRO2NO*AlkNitrate6*1.0*1.0)
k[EPOXY2PROPO --> METHACETO2]=CONST(KDEC)
k[EPOXY2PROPO2+HO2-->EPOXY2PROPOOH]=CONST(KRO2HO2*0.387)
k[EPOXY2PROPO2+NO3-->METHACETO2+NO2]=CONST(KRO2NO3)
k[EPOXY2PROPO2-->METHACETO2]=CONST(8.8D-13*RO2)
k[EPOXY2PROPOOH+OH-->EPOXY2PROPO2]=CONST(7.15D-12)
k[EPOXY2PROPOOH+hv-->METHACETO2+OH]=CONST(J41)
```

```
;FROM MCM
k[METHACETO2+HO2-->METACETHO]=CONST(KRO2HO2*0.520*0.4)
k[METHACETO2+HO2-->METACETO2H]=CONST(KRO2HO2*0.520*0.6)
k[METHACETO2+NO-->METACETNO3]=CONST(KRO2NO*0.019)
k[METHACETO2+NO-->METHACETO+NO2]=CONST(KRO2NO*0.981)
k[METHACETO2+NO3-->METHACETO+NO2]=CONST(KRO2NO3)
k[METHACETO2-->METACETHO]=CONST(2.00D-12*0.2*RO2)
k[METHACETO2-->METACETOH]=CONST(2.00D-12*0.2*RO2)
k[METHACETO2-->METHACETO]=CONST(2.00D-12*0.6*RO2)
k[METACETHO+OH-->CH3CO3]=CONST(9.82D-11)
k[METACETO2H+OH-->METACETHO+OH]=CONST(6.65D-11)
k[METACETO2H+OH-->METHACETO2]=CONST(1.90D-12*EXP(190/(T)))
k[METACETO2H+hv-->METHACETO+OH]=CONST(J41)
k[METACETNO3+OH-->METACETHO+NO2]=CONST(2.26D-13)
k[METACETNO3+hv-->METHACETO+NO2]=CONST(J53)
k[METHACETO-->HCHO+CH3O2]=CONST(KDEC)
k[METACETOH+OH-->METACETHO+HO2]=CONST(1.74D-11)

;############
; Updated isoprene ozonolysis chemistry
;############
k[O3+C5H8-->CH2OOE+MACR]=CONST(1.03D-14*EXP(-1995/(T))*0.6*0.68)
k[O3+C5H8-->HCHO+EMACROOA]=CONST(1.03D-14*EXP(-1995/(T))*0.6*0.32*0.79)
k[O3+C5H8-->HCHO+ZMACROOA]=CONST(1.03D-14*EXP(-1995/(T))*0.6*0.32*0.21)
k[O3+C5H8-->CH2OOE+MVK]=CONST(1.03D-14*EXP(-1995/(T))*0.4*0.42)
k[O3+C5H8-->HCHO+EMVKOOA]=CONST(1.03D-14*EXP(-1995/(T))*0.4*0.58*0.60)
k[O3+C5H8-->HCHO+ZMVKOOA]=CONST(1.03D-14*EXP(-1995/(T))*0.4*0.58*0.40)
k[ZMACROOA-->IBUTDIAL]=CONST(KDEC)
k[EMACROOA-->MACO2H]=CONST(KDEC*0.333)
k[EMACROOA-->C3H6]=CONST(KDEC*0.333)
k[EMACROOA-->CH3COCH3]=CONST(KDEC*0.167)
k[EMACROOA-->CH3C2H2O2+HO2]=CONST(KDEC*0.167)
k[ZMVKOOA-->CO2C3CHO]=CONST(KDEC)
k[EMVKOOA-->OH+MVKO2]=CONST(KDEC)
k[CH2OOE-->CH2OO]=CONST(KDEC*1.0)  ; assume all CH2OO is stabilized
; CH2OO scavenging by CO and NO2 as in Novelli et al., PCCP, 2021
k[CH2OO+CO-->HCHO+CO2]=CONST(1.00D-15)
k[CH2OO+NO2-->CH2NO2O2]=CONST(3.00D-12)
k[CH2NO2O2 + NO --> CH2NO2O + NO2] = CONST(2.7D-12*exp(360./T))
k[CH2NO2O2 + NO3 --> CH2NO2O + NO2] = CONST(1.9E-11*EXP(-390/T))
k[CH2NO2O2 + HO2 --> CH2NO2OOH] = CONST(1.7D-13*exp(1300./T))
k[CH2NO2O2 + RO2 --> CH2NO2O] = CONST(2.0E-12*0.6)
k[CH2NO2O2 + RO2 --> CH2NO2OH] = CONST(2.0E-12*0.2)
k[CH2NO2O2 + RO2 --> CH2NO2CO] = CONST(2.0E-12*0.2)
k[CH2NO2O --> HCHO + NO2 ] = CONST(KDEC)
; CH2OO scavenging by NO and SO2 as IUPAC 2020 and Vereecken et al. 2012
k[CH2OO+NO-->HCHO+NO2]=CONST(1.70D-18)
k[CH2OO+SO2-->HCHO+SO3]=CONST(3.70D-11)
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; Scavenging by water and acids not included

;############
; Updated propene ozonolysis as in Novelli et al., PCCP, 2021
;############
k[O3+C3H6-->CH2OOB+CH3CHO]=CONST(5.5D-15*EXP(-1880/(T))*0.38)
k[O3+C3H6-->ZCH3CHOO+HCHO]=CONST(5.5D-15*EXP(-1880/(T))*0.62*0.58)
k[O3+C3H6-->ECH3CHOO+HCHO]=CONST(5.5D-15*EXP(-1880/(T))*0.62*0.42)
k[CH2OOB-->CH2OO]=CONST(KDEC*0.6)
k[CH2OOB-->H2 + CO2]=CONST(KDEC*0.4*0.43)
k[CH2OOB-->CO + H2O]=CONST(KDEC*0.4*0.43)
k[CH2OOB-->HO2 + HO2 + CO2]=CONST(KDEC*0.4*14)
k[ZCH3CHOO-->HCOCH2O2+OH]=CONST(KDEC)
k[ECH3CHOO-->CH3CO2H]=CONST(KDEC*0.09)
k[ECH3CHOO-->CH4 + CO2]=CONST(KDEC*0.41)
k[ECH3CHOO-->CH3OH+CO]=CONST(KDEC*0.23)
k[ECH3CHOO-->H2CCO]=CONST(KDEC*0.0)
k[ECH3CHOO-->CH3O2+HO2+CO2]=CONST(KDEC*0.27)

;############
; Additional HCOCH2O2 chemistry from Novelli et al. PCCP, 2021
;############
; H-shift and alkyl radical chemistry
k[HCOCH2O2 --> COCH2OOH]=CONST(2.07E-70*T@(26.14)*EXP(2471/T))
k[COCH2OOH --> HCHO+CO+OH]=CONST(2.27E+12*T@(0.47)*EXP(-5529/T))
k[COCH2OOH + O2 --> HOOCH2CO3]=CONST(7.50D-12)
; acylperoxy radical chemistry
k[HOOCH2CO3 --> CO3HCH2O2]=CONST(2.94E-35*T@(13.82)*EXP(2222/T))
k[HOOCH2CO3+HO2 --> HO2CH2CO3H]=CONST(KAPHO2*0.41)
k[HOOCH2CO3+HO2 --> OH+HOOCH2CO2]=CONST(KAPHO2*0.44)
k[HOOCH2CO3+HO2 --> O3+HOOCH2CO2H]=CONST(KAPHO2*0.15)
k[HOOCH2CO3+NO3 --> OCOCH2OOH + NO2]=CONST(KRO2NO3*1.74)
k[HOOCH2CO3+RO2 --> HOOCH2CO2]=CONST(1.0D-11*0.7)
k[HOOCH2CO3+RO2 --> HOOCOCH2OOH]=CONST(1.0D-11*0.3)
k[HOOCH2CO3+NO --> HOOCH2CO2 + NO2]=CONST(KAPNO)
k[HOOCH2CO3+NO2 --> HOOCH2CO3NO2]=CONST(KFPAN)
k[HOOCH2CO3NO2 --> NO2 + HOOCH2CO3]=CONST(KBPAN)
k[HOOCH2CO2 --> CO2 + HCHO + OH]=CONST(KDEC)
; peracid-RO2 radical chemistry
k[CO3HCH2O2 --> HOOCH2CO3]=CONST(2.98E-41*T@(15.62)*EXP(-135./T))
k[CO3HCH2O2+HO2 --> HO2CH2CO3H]=CONST(SARRO2HO2_5NOC)
k[CO3HCH2O2+NO3 --> CO3HCH2O + NO2]=CONST(1.6E-11*EXP(-480./T))
k[CO3HCH2O2+RO2 --> CO3HCH2O]=CONST(1.0E-13*EXP(983./T)*0.6)
k[CO3HCH2O2+RO2 --> HCOCO3H]=CONST(1.0E-13*EXP(983./T)*0.2)
k[CO3HCH2O2+RO2 --> HOCH2CO3H]=CONST(1.0E-13*EXP(983./T)*0.2)
k[CO3HCH2O2+NO --> CO3HCH2O]=CONST(KRO2NO*(1-AlkNitrate5*0.3*0.65))
k[CO3HCH2O2+NO --> CO3HCH2NO3]=CONST(KRO2NO*AlkNitrate5*0.3*0.65)
; peracid-RO radical chemistry
```

```
k[CO3HCH2O --> HO + CO2 + HCHO]=CONST(1.34E-03*T@(5.55)*EXP(-6947/T))
k[CO3HCH2O --> HOCH2CO3]=CONST(1.31E-38*T@(16.18)*EXP(4812./T))
k[CO3HCH2O+O2 --> HCOCO3H + HO2]=CONST(KROPRIM)


;############
; Additional NO3-propene-OO chemistry
;############
yield_alkoxy=CONST(0.52)
k[PRONO3AO2+HO2-->PR1O2HNO3]=CONST(KRO2HO2*0.520*(1-yield_alkoxy))
k[PRONO3AO2+HO2-->PRONO3AO+OH]=CONST(KRO2HO2*0.520*yield_alkoxy)
k[PRONO3BO2+HO2-->PR2O2HNO3]=CONST(KRO2HO2*0.520*(1-yield_alkoxy))
k[PRONO3BO2+HO2-->PRONO3BO+OH]=CONST(KRO2HO2*0.520*yield_alkoxy)
k[PRONO3AO-->HCHO+CH3CHO+NO2]=CONST((1.11e8*T@(1.74)*EXP(-6379/T)))
k[PRONO3BO-->CH3CHO+HCHO+NO2]=CONST((2.40e9*T@(1.41)*EXP(-6950/T)))


;############
; Remaining chemistry imported from CalTech model
;############

k[ISOP1N2OOH + OH --> ISOP1N2OOH3R4OH ] = CONST(8.38E-12*EXP(390./T)*0.75)
k[ISOP1N2OOH3R4OH + O2 --> ISOP1N2OOH3OO4OH ] = CONST(1.0E-14)
k[ISOP1N2OOH3R4OH --> ISOP1N23O4OH + OH ] = CONST(9.2E4)
k[ISOP1N2OOH + OH --> ISOP1N2OOH3OH4OO ] = CONST(8.38E-12*EXP(390./T)*0.25)
k[ISOP1N4OOH + OH --> ISOP1N2OH3R4OOH ] = CONST(2.24E-11*EXP(390./T)*0.3)
k[ISOP1N2OH3R4OOH + O2 --> ISOP1N2OH3OO4OOH ] = CONST(1.0E-14)
k[ISOP1N2OH3R4OOH --> ISOP1N2OH34O + OH ] = CONST(9.61E4)
k[ISOP1N4OOH + OH --> ISOP1N2R3OH4OOH ] = CONST(2.24E-11*EXP(390./T)*0.7)
k[ISOP1N2R3OH4OOH + O2 --> ISOP1N2OO3OH4OOH ] = CONST(1.0E-14)
k[ISOP1N2R3OH4OOH --> ISOP12O3OH4OOH +  NO2 ] = CONST(7.73E3)
k[ISOP3OOH4N + OH --> ISOP1OH2R3OOH4N ] = CONST(1.17E-11*EXP(390./T)*0.9)
k[ISOP1OH2R3OOH4N + O2 --> ISOP1OH2OO3OOH4N ] = CONST(1.0E-14)
k[ISOP1OH2R3OOH4N --> ISOP1OH23O4N + OH ] = CONST(9.2E4)
k[ISOP3OOH4N + OH --> ISOP1OO2OH3OOH4N ] = CONST(1.17E-11*EXP(390./T)*0.1)
k[ISOP1OOH4N + OH --> ISOP1OOH2R3OH4N ] = CONST(3.07E-11*EXP(390./T)*0.7)
k[ISOP1OOH2R3OH4N + O2 --> ISOP1OOH2OO3OH4N ] = CONST(1.0E-14)
k[ISOP1OOH2R3OH4N --> ISOP12O3OH4N + OH ] = CONST(9.61E4)
k[ISOP1OOH4N + OH --> ISOP1OOH2OH3R4N ] = CONST(3.07E-11*EXP(390./T)*0.3)
k[ISOP1OOH2OH3R4N + O2 --> ISOP1OOH2OH3OO4N ] = CONST(1.0E-14)
k[ISOP1OOH2OH3R4N --> ISOP1OOH2OH34O + NO2 ] = CONST(7.73E3)
k[ISOP1N2OOH + OH --> ISOP1N2OO + H2O ] = CONST(3.4E-12*EXP(200./T))
k[ISOP1N4OOH + OH --> EISOP1N4OO + H2O ] = CONST(3.4E-12*EXP(200./T))
k[ISOP3OOH4N + OH --> ISOP3OO4N + H2O ] = CONST(3.4E-12*EXP(200./T))
k[ISOP1OOH4N + OH --> EISOP1OO4N + H2O ] = CONST(3.4E-12*EXP(200./T))
k[ISOP1N4OOH + OH --> OH + ISOP1N4CO ] = CONST(7.5E-12*EXP(20./T))
k[ISOP1OOH4N + OH --> OH + ISOP1CO4N ] = CONST(7.5E-12*EXP(20./T))
k[ISOP3OOH4N + OH --> OH + ISOP3CO4N ] = CONST(7.5E-12*EXP(20./T))
k[ISOP1N2OOH3OO4OH + NO --> ISOP1N2OOH3N4OH ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1N2OOH3OO4OH + NO --> NO2 + NOA + HOCH2CHO + OH ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.8)
k[ISOP1N2OOH3OO4OH + NO --> NO2 + HO2 + HCHO + MACR2OOH3N ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.2)
k[ISOP1N2OOH3OH4OO + NO --> ISOP1N2OOH3OH4N ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1N2OOH3OH4OO + NO --> NO2 + HO2 + HCHO + MACR2OOH3N ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*0.65))
k[ISOP1N2OH3OO4OOH + NO --> ISOP1N2OH3N4OOH ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1N2OH3OO4OOH + NO --> NO2 + MACRNB + HCHO + OH ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.8)
k[ISOP1N2OH3OO4OOH + NO --> NO2 + NOA + HCOCH2OOH + HO2 ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.2)
k[ISOP1N2OO3OH4OOH + NO --> ISOP1N2N3OH4OOH ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
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k[ISOP1N2OO3OH4OOH + NO --> NO2 + NOA + HCOCH2OOH + HO2 ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0))
k[ISOP1OH2OO3OOH4N + NO --> ISOP1OH2N3OOH4N ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1OH2OO3OOH4N + NO --> NO2 + HO2 + HCHO + MVK3OOH4N ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.2)
k[ISOP1OH2OO3OOH4N + NO --> NO2 + ACETOL + NO3CH2CHO + OH ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.8)
k[ISOP1OO2OH3OOH4N + NO --> ISOP1N2OH3OOH4N ] = CONST(KRO2NO*AlkNitrate12*0.65*0.65)
k[ISOP1OO2OH3OOH4N + NO --> HO2 + NO2 + HCHO + MVK3OOH4N ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*0.65))
k[ISOP1OOH2OO3OH4N + NO --> ISOP1OOH2N3OH4N ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1OOH2OO3OH4N + NO --> NO2 + HYPERACET + NO3CH2CHO + HO2 ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.8)
k[ISOP1OOH2OO3OH4N + NO --> NO2 + HMVKANO3 + HCHO + OH ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.2)
k[ISOP1OOH2OH3OO4N + NO --> ISOP1OOH2OH3N4N ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1OOH2OH3OO4N + NO --> NO2 + HYPERACET + NO3CH2CHO + HO2 ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0))
k[ISOP1OOH2OH3OO4N + HO2 --> OH + HYPERACET + NO3CH2CHO + HO2 ] = CONST(0.75*2.64E-13*EXP(1300./T))
k[ISOP1OOH2OH3OO4N + HO2 --> ISOP1OOH2OH3OOH4N ] = CONST(0.25*2.64E-13*EXP(1300./T))
k[ISOP1N2OOH3OO4OH --> ISOP1N2OO3OOH4OH ] = CONST(4.0E6)
k[ISOP1N2OOH3OH4OO --> ISOP1N2OO3OH4OOH ] = CONST(4.0E6)
k[ISOP1N2OH3OO4OOH --> ISOP1N2OH3OOH4OO ] = CONST(2.0E6)
k[ISOP1N2OO3OH4OOH --> ISOP1N2OOH3OH4OO ] = CONST(2.0E6)
k[ISOP1OH2OO3OOH4N --> ISOP1OH2OOH3OO4N ] = CONST(3.0E6)
k[ISOP1OO2OH3OOH4N --> ISOP1OOH2OH3OO4N ] = CONST(3.0E6)
k[ISOP1OOH2OO3OH4N --> ISOP1OO2OOH3OH4N ] = CONST(2.0E6)
k[ISOP1OOH2OH3OO4N --> ISOP1OO2OH3OOH4N ] = CONST(2.0E6)
k[ISOP1N2OO3OOH4OH --> ISOP1N2OOH3OO4OH ] = CONST(3.0E6)
k[ISOP1N2OH3OOH4OO --> ISOP1N2OH3OO4OOH ] = CONST(3.0E6)
k[ISOP1OH2OOH3OO4N --> ISOP1OH2OO3OOH4N ] = CONST(4.0E6)
k[ISOP1OO2OOH3OH4N --> ISOP1OOH2OO3OH4N ] = CONST(4.0E6)
k[ISOP1N2OO3OOH4OH + HO2 --> HMVKBOOH + NO2 + HCHO + OH ] = CONST(0.2*2.64E-13*EXP(1300./T))
k[ISOP1N2OO3OOH4OH + HO2 --> OH + OH + HOCH2CHO + NOA ] = CONST(0.8*2.64E-13*EXP(1300./T))
k[ISOP1N2OO3OOH4OH + NO --> ISOP1N2N3OOH4OH ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1N2OO3OOH4OH + NO --> HMVKBOOH + NO2 + NO2 + HCHO ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.2)
k[ISOP1N2OO3OOH4OH + NO --> NO2 + OH + HOCH2CHO + NOA ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.8)
k[ISOP1N2OH3OOH4OO + NO --> ISOP1N2OH3OOH4N ] = CONST(KRO2NO*AlkNitrate12*0.65*0.65)
k[ISOP1N2OH3OOH4OO + NO --> MACRNB + OH + NO2 + HCHO ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*0.65))
k[ISOP1OH2OOH3OO4N + HO2 --> ISOP1OH2OOH3OOH4N ] = CONST(0.25*2.64E-13*EXP(1300./T))
k[ISOP1OH2OOH3OO4N + HO2 --> MACR2OOH3OH + OH + NO2 + HCHO ] = CONST(0.15*2.64E-13*EXP(1300./T))
k[ISOP1OH2OOH3OO4N + HO2 --> ACETOL + NO3CH2CHO + OH + OH ] = CONST(0.6*2.64E-13*EXP(1300./T))
k[ISOP1OH2OOH3OO4N + NO --> ISOP1OH2OOH3N4N ] = CONST(KRO2NO*AlkNitrate12*0.65*1.0)
k[ISOP1OH2OOH3OO4N + NO --> MACR2OOH3OH + NO2 + NO2 + HCHO ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.2)
k[ISOP1OH2OOH3OO4N + NO --> ACETOL + NO3CH2CHO + OH + NO2] = CONST(KRO2NO*(1-AlkNitrate12*0.65*1.0)*0.8)
k[ISOP1OO2OOH3OH4N + NO --> ISOP1N2OOH3OH4N ] = CONST(KRO2NO*AlkNitrate12*0.65*0.65)
k[ISOP1OO2OOH3OH4N + NO --> HMVKANO3 + OH + NO2 + HCHO ] = CONST(KRO2NO*(1-AlkNitrate12*0.65*0.65))
k[ISOP1N2OO3OH4OOH --> ISOP1N2OOH3OH4CO + OH ] = CONST(9.375E12*EXP(-10000./T))
k[ISOP1OOH2OH3OO4N --> ISOP1CO2OH3OOH4N + OH ] = CONST(9.375E12*EXP(-10000./T))
k[ISOP1OO2OOH3OH4N --> ISOP1OOH23O3OH4N + OH ] = CONST(3.75E13*EXP(-10000./T))
k[ISOP1N2OO3OOH4OH --> ISOP1N2OOH34O4OH + OH ] = CONST(1.875E13*EXP(-10000./T))
k[ISOP1OO2OH3OOH4N --> ISOP1OOH2OH3CO4N + OH ] = CONST(1.875E13*EXP(-10000./T))
k[ISOP1OH2OOH3OO4N --> ISOP1OH12O3OOH4N + OH ] = CONST(1.875E13*EXP(-10000./T))
k[ISOP1N23O4OH + OH --> ISOP1N23O4OH4R ] = CONST(4.78E-11*EXP(-400./T))
k[ISOP1N23O4OH4R + O2 --> ISOP1N23O4CO + HO2 ] = CONST(1.0E-14)
k[ISOP1N23O4OH4R --> HCHO + NO2 + HVMK ] = CONST(0.5*2.07E5)
k[ISOP1N23O4OH4R --> ISOP1N2OH3OO4CO ] = CONST(0.5*2.07E5)
k[ISOP1OH23O4N + OH --> ISOP1OH1R23O4N ] = CONST(4.78E-11*EXP(-400./T))
k[ISOP1OH1R23O4N + O2 --> ISOP1CO23O4N + HO2 ] = CONST(1.0E-14)
k[ISOP1OH1R23O4N --> HCHO + NO2 + HMAC ] = CONST(0.5*2.07E5)
k[ISOP1OH1R23O4N --> ISOP1CO2OO3OH4N ] = CONST(0.5*2.07E5)
k[ISOP1N2OH34O + OH --> ISOP1N2OH3OO4CO ] = CONST(0.5*3.22E-11*EXP(-400./T))
k[ISOP1N2OH34O + OH --> ISOP1N2OH3CO4OO ] = CONST(0.5*3.22E-11*EXP(-400./T))
k[ISOP12O3OH4N + OH --> ISOP12O3OH3R4N ] = CONST(3.22E-11*EXP(-400./T))
k[ISOP12O3OH3R4N + O2 --> ISOP12O3CO4N + HO2 ] = CONST(1.0E-14)
k[ISOP12O3OH3R4N --> ISOP1OH2OO3CO4N ] = CONST(2.07E5)
k[ISOP1N2OH3CO4OO + NO --> ISOP1N2OH3CO4N ] = CONST(KRO2NO*AlkNitrate11*0.65*0.3)
k[ISOP1N2OH3CO4OO + NO --> NOA + CO + HO2 + HCHO + NO2 ] = CONST(KRO2NO*(1-AlkNitrate11*0.65*0.3))
k[ISOP3CO4N + OH --> ISOP1OH2OO3CO4N ] = CONST(2.7E-12*EXP(390./T))
k[ISOP1OH2OO3CO4N + NO --> CO2C4NO3 + NO2 + HO2 + HCHO ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3)*0.8)
k[ISOP1OH2OO3CO4N + NO --> ISOP1OH2N3CO4N ] = CONST(KRO2NO*AlkNitrate11*1.0*0.3)
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k[ISOP1OH2OO3CO4N + NO --> ACETOL + NO2 + NO3CH2CO3 ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3)*0.2)
k[ISOP1N2OO3CO4OH + NO --> ISOP1N2N3CO4OH ] = CONST(KRO2NO*AlkNitrate11*1.0*0.3)
k[ISOP1N2OO3CO4OH + NO --> NO2 + NOA + CH3CO3 ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3))
k[ISOP1N2OO3CO4OH + HO2 --> OH + NOA + CH3CO3 ] = CONST(2.6E-13*EXP(1300./T))
k[ISOP1N4CO + OH --> ISOP1N4R4CO ] = CONST(3.3E-12*EXP(470./T))
k[ISOP1N4R4CO + O2 --> ISOP1N4CO4OO ] = CONST(1.0E-14)
k[ISOP1N4CO4OO + NO2 --> ISOP1N4PAN  ] = COMPRC( 2.591*M*(T/300)@(-6.87), 1.125D-11*(T/300)@(-1.105), 0.3)
k[ISOP1N4CO4OO + NO --> NO2 + CO2 + C4NVP2 ] = CONST(2.7E-12*EXP(350./T))
k[ISOP1N4CO4OO + HO2 --> ISOP1N4CO4OOH ] = CONST(3.14E-12*EXP(580./T)*0.37)
k[ISOP1N4CO4OO + HO2 --> O3 + ISOP1N4CO4OH ] = CONST(3.14E-12*EXP(580./T)*0.13)
k[ISOP1N4CO4OO + HO2 --> OH + CO2 + C4NVP2 ] = CONST(3.14E-12*EXP(580./T)*0.5)
k[C4NVP2 + NO --> NO2 + MACR2OO3N ] = CONST(2.7E-12*EXP(350./T))
k[C4NVP2 + HO2 --> OH + MACR2OO3N ] = CONST(2.38E-13*EXP(1300./T))
k[C4NVP2 + NO2 --> MACR2N3N ] = CONST(9.0E-12)
k[MACR2OO3N --> CO + OH + NOA ] = CONST(1.0E7*EXP(-5000./T))
k[MACR2OO3N + NO --> NO2 + HO2 + CO + NOA ] = CONST(2.7E-12*EXP(350./T))
k[MACR2OO3N + HO2 --> OH + HO2 + CO + NOA ] = CONST(2.8E-13*EXP(1300./T)*0.87)
k[ISOP1N4PAN --> ISOP1N4CO4OO + NO2  ] = CONST(1.58E16*EXP(-13500./T))
k[ISOP1CO4N + OH --> ISOP1CO1R4N ] = CONST(3.3E-12*EXP(470./T))
k[ISOP1CO1R4N + O2 --> ISOP1CO1OO4N ] = CONST(1.0E-14)
k[ISOP1CO1OO4N + NO2 --> ISOP1PAN4N  ] = COMPRC( 2.591*M*(T/300)@(-6.87), 1.125D-11*(T/300)@(-1.105), 0.3)
k[ISOP1CO1OO4N + NO --> NO2 + CO2 + C4NVP1 ] = CONST(2.7E-12*EXP(350./T))
k[ISOP1CO1OO4N + HO2 --> ISOP1CO1OOH4N ] = CONST(3.14E-12*EXP(580./T)*0.37)
k[ISOP1CO1OO4N + HO2 --> O3 + ISOP1CO1OH4N ] = CONST(3.14E-12*EXP(580./T)*0.13)
k[ISOP1CO1OO4N + HO2 --> OH + CO2 + C4NVP1 ] = CONST(3.14E-12*EXP(580./T)*0.5)
k[C4NVP1 + NO --> NO2 + MVK3OO4N ] = CONST(2.7E-12*EXP(350./T))
k[C4NVP1 + HO2 --> OH + MVK3OO4N ] = CONST(2.38E-13*EXP(1300./T))
k[C4NVP1 + NO2 --> MVK3N4N ] = CONST(9.0E-12)
k[MVK3OO4N + NO --> NO2 + NO3CH2CHO + CH3CO3 ] = CONST(2.7E-12*EXP(350./T))
k[MVK3OO4N + HO2 --> OH + NO3CH2CHO + CH3CO3 ] = CONST(2.8E-13*EXP(1300./T)*0.87)
k[ISOP1PAN4N --> ISOP1CO1OO4N + NO2  ] = CONST(1.58E16*EXP(-13500./T))
k[ISOP1N4CO + OH --> ISOP1N2R3OH4CO ] = CONST(4.86E-12*EXP(390./T)*0.7)
k[ISOP1N2R3OH4CO + O2 --> ISOP1N2OO3OH4CO ] = CONST(1.0E-14)
k[ISOP1N2R3OH4CO --> ISOP12O3OH4CO + NO2 ] = CONST(7.73E3)
k[ISOP1N4CO + OH -->  ISOP1N2OH3OO4CO ] = CONST(4.86E-12*EXP(390./T)*0.3)
k[ISOP1CO4N + OH --> ISOP1CO2OH3R4N ] = CONST(6.75E-12*EXP(390./T)*0.3)
k[ISOP1CO2OH3R4N + O2 --> ISOP1CO2OH3OO4N ] = CONST(1.0E-14)
k[ISOP1CO2OH3R4N --> ISOP1CO2OH34O + NO2 ] = CONST(7.73E3)
k[ISOP1CO4N + OH --> ISOP1CO2OO3OH4N ] = CONST(6.75E-12*EXP(390./T)*0.7)
k[ISOP1N2OO3OH4CO --> MACR2OOH3N + CO + HO2 ] = CONST(4.0E8*EXP(-5000./T))
k[ISOP1CO2OH3OO4N --> MVK3OOH4N + CO + HO2 ] = CONST(4.0E8*EXP(-5000./T))
k[ISOP1N2OH3OO4CO --> MACRNB + CO + OH ] = CONST(1.0E7*EXP(-5000./T))
k[ISOP1N2OH3OO4CO + NO --> ISOP1N2OH3N4CO ] = CONST(KRO2NO*AlkNitrate11*1.0*0.3)
k[ISOP1N2OH3OO4CO + NO --> MACRNB + NO2 + HO2 + CO  ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3)*0.8)
k[ISOP1N2OH3OO4CO + NO --> NO2 + HO2 + NOA + GLYOX ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3)*0.2)
k[ISOP1CO2OO3OH4N --> HMVKANO3 + CO + OH ] = CONST(1.0E7*EXP(-5000./T))
k[ISOP1CO2OO3OH4N + NO --> HMVKANO3 + NO2 + HO2 + CO ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3)*0.8)
k[ISOP1CO2OO3OH4N + NO --> NO2 + HO2 + MGLYOX + NO3CH2CHO] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.3)*0.2)
k[ISOP1CO2OO3OH4N + NO --> ISOP1CO2N3OH4N ] = CONST(KRO2NO*AlkNitrate11*1.0*0.3)
k[ISOP1N2OH + OH --> ISOP1N2OH3OO4OH ] = CONST(8.38E-12*EXP(390./T)*0.75)
k[ISOP1N2OH + OH --> ISOP1N2OH3OH4OO ] = CONST(8.38E-12*EXP(390./T)*0.25)
k[ZISOP1N4OH + OH --> ISOP1N2R3OH4OH ] = CONST(2.24E-11*EXP(390./T)*0.7)
k[EISOP1N4OH + OH --> ISOP1N2R3OH4OH ] = CONST(2.24E-11*EXP(390./T)*0.7)
k[ISOP1N2R3OH4OH + O2 --> ISOP1N2OO3OH4OH ] = CONST(1.0E-14)
k[ISOP1N2R3OH4OH --> ISOP12O3OH4OH ] = CONST(7.73E3)
k[ZISOP1N4OH + OH --> ISOP1N2OH3OO4OH ] = CONST(2.24E-11*EXP(390./T)*0.3)
k[EISOP1N4OH + OH --> ISOP1N2OH3OO4OH ] = CONST(2.24E-11*EXP(390./T)*0.3)
k[ISOP3OH4N + OH --> ISOP1OH2OO3OH4N ] = CONST(1.17E-11*EXP(390./T)*0.9)
k[ISOP3OH4N + OH --> ISOP1OO2OH3OH4N ] = CONST(1.17E-11*EXP(390./T)*0.1)
k[ZISOP1OH4N + OH --> ISOP1OH2OH3R4N ] = CONST(3.07E-11*EXP(390./T)*0.3)
k[EISOP1OH4N + OH --> ISOP1OH2OH3R4N ] = CONST(3.07E-11*EXP(390./T)*0.3)
k[ISOP1OH2OH3R4N + O2 --> ISOP1OH2OH3OO4N ] = CONST(1.0E-14)
k[ISOP1OH2OH3R4N --> ISOP1OH2OH34O ] = CONST(7.73E3)
k[ZISOP1OH4N + OH --> ISOP1OH2OO3OH4N ] = CONST(3.07E-11*EXP(390./T)*0.7)
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k[EISOP1OH4N + OH --> ISOP1OH2OO3OH4N ] = CONST(3.07E-11*EXP(390./T)*0.7)
k[ISOP1OH2OH3OO4N --> ISOP1CO2OH3OOH4N + HO2 ] = CONST(1.875E13*EXP(-10000./T))
k[ISOP1N2OO3OH4OH --> ISOP1N2OOH3OH4CO + HO2 ] = CONST(1.875E13*EXP(-10000./T))
k[ISOP1N2OO3OH4OH + HO2 --> ISOP1N2OOH3OH4OH ] = CONST(2.6E-13*EXP(1300./T)*0.35)
k[ISOP1N2OO3OH4OH + HO2 --> OH + HO2 + NOA + HOCH2CHO  ] = CONST(2.6E-13*EXP(1300./T)*0.65)
k[ISOP1OH2OH3OO4N + HO2 --> ISOP1OH2OH3OOH4N ] = CONST(2.6E-13*EXP(1300./T)*0.35)
k[ISOP1OH2OH3OO4N + HO2 --> OH + HO2 + ACETOL + NO3CH2CHO ] = CONST(2.6E-13*EXP(1300./T)*0.65)
k[ISOP1N2OO3OH4OH + NO --> ISOP1N2N3OH4OH ] = CONST(KRO2NO*AlkNitrate11*1.0*0.65)
k[ISOP1N2OO3OH4OH + NO --> NO2 + HO2 + NOA + HOCH2CHO ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.65))
k[ISOP1N2OH3OO4OH + NO --> ISOP1N2OH3N4OH ] = CONST(KRO2NO*AlkNitrate11*1.0*0.65)
k[ISOP1N2OH3OO4OH + NO --> MACRNB + HCHO + HO2 + NO2 ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.65)*0.2)
k[ISOP1N2OH3OO4OH + NO --> NO2 + HO2 + NOA + HOCH2CHO ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.65)*0.8)
k[ISOP1OH2OH3OO4N + NO --> ISOP1OH2OH3N4N ] = CONST(KRO2NO*AlkNitrate11*1.0*0.65)
k[ISOP1OH2OH3OO4N + NO --> NO2 + HO2 + ACETOL + NO3CH2CHO ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.65))
k[ISOP1OH2OO3OH4N + NO --> ISOP1OH2N3OH4N ] = CONST(KRO2NO*AlkNitrate11*1.0*0.65)
k[ISOP1OH2OO3OH4N + NO --> HMVKANO3 + HCHO + HO2 + NO2 ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.65)*0.2)
k[ISOP1OH2OO3OH4N + NO --> NO2 + HO2 + ACETOL + NO3CH2CHO ] = CONST(KRO2NO*(1-AlkNitrate11*1.0*0.65)*0.8)
k[ISOP1OO2OH3OH4N --> ISOP1OOH2OH3CO4N + HO2 ] = CONST(3.75E13*EXP(-10000./T))
k[ISOP1N2OH3OH4OO + NO --> ISOP1N2OH3OH4N ] = CONST(KRO2NO*AlkNitrate11*0.65*0.65)
k[ISOP1N2OH3OH4OO + NO --> HO2 + NO2 + HCHO + MACRNB ] = CONST(KRO2NO*(1-AlkNitrate11*0.65*0.65))
k[ISOP1OO2OH3OH4N + NO --> ISOP1N2OH3OH4N ] = CONST(KRO2NO*AlkNitrate11*0.65*0.65)
k[ISOP1OO2OH3OH4N + NO --> HO2 + NO2 + HCHO + HMVKANO3 ] = CONST(KRO2NO*(1-AlkNitrate11*0.65*0.65))
k[ZISOP1N4OH + OH --> ISOP1N4R4OH ] = CONST(7.5E-12*EXP(20./T))
k[EISOP1N4OH + OH --> ISOP1N4R4OH ] = CONST(7.5E-12*EXP(20./T))
k[ISOP1N4R4OH + O2 --> ISOP1N4CO + HO2 ] = CONST(0.4*1.0E-14)
k[ISOP1N4R4OH + O2 --> ISOP1N2OOH3OO4CO ] = CONST(0.6*1.0E-14)
k[ISOP1N2OOH3OO4CO --> ISOP1N2OO3OOH4CO ] = CONST(4.E6)
k[ISOP1N2OO3OOH4CO --> ISOP1N2OOH3OO4CO ] = CONST(3.E6)
k[ISOP1N2OO3OOH4CO --> OH + CO + MACR2OOH3N ] = CONST(4.0E8*EXP(-5000./T))
k[ISOP1N2OOH3OO4CO --> OH + CO + MACR2OOH3N ] = CONST(1.0E7*EXP(-5000./T))
k[ZISOP1OH4N + OH --> ISOP1OH1R4N ] = CONST(7.5E-12*EXP(20./T))
k[EISOP1OH4N + OH --> ISOP1OH1R4N ] = CONST(7.5E-12*EXP(20./T))
k[ISOP1OH1R4N + O2 --> ISOP1CO4N + HO2 ] = CONST(0.4*1.0E-14)
k[ISOP1OH1R4N + O2 --> ISOP1CO2OO3OOH4N ] = CONST(0.6*1.0E-14)
k[ISOP1CO2OO3OOH4N --> ISOP1CO2OOH3OO4N ] = CONST(3.E6)
k[ISOP1CO2OOH3OO4N --> ISOP1CO2OO3OOH4N ] = CONST(4.E6)
k[ISOP1CO2OO3OOH4N --> OH + CO + MVK3OOH4N ] = CONST(1.0E7*EXP(-5000./T))
k[ISOP1CO2OOH3OO4N --> OH + CO + MVK3OOH4N ] = CONST(4.0E8*EXP(-5000./T))
k[ISOP3OH4N + OH --> ISOP3OH3R4N ] = CONST(7.5E-12*EXP(20./T))
k[ISOP3OH3R4N + O2 --> ISOP3CO4N + HO2 ] = CONST(0.6*1.0E-14)
k[ISOP3OH3R4N + O2 --> ISOP1OOH2R3CO4N ] = CONST(0.4*1.0E-14)
k[ISOP1OOH2R3CO4N --> OH + ISOP12O3CO4N ] = CONST(1.0E3)

;#############
; Remaining chemistry imported from MCM v3.3.1
;#############
k[OH+C5H8-->CISOPA]=CONST(2.70D-11*EXP(390/(T))*0.288)
k[OH+C5H8-->CISOPC]=CONST(2.70D-11*EXP(390/(T))*0.238)
k[OH+C5H8-->ISOP34O2]=CONST(2.70D-11*EXP(390/(T))*0.022)
k[OH+C5H8-->ME3BU3ECHO+HO2]=CONST(2.70D-11*EXP(390/(T))*0.020)
k[OH+C5H8-->PE4E2CO+HO2]=CONST(2.70D-11*EXP(390/(T))*0.042)
k[OH+C5H8-->TISOPA]=CONST(2.70D-11*EXP(390/(T))*0.288)
k[OH+C5H8-->TISOPC]=CONST(2.70D-11*EXP(390/(T))*0.102)
k[MACR+hv-->CH3C2H2O2+CO+HO2]=CONST(J18)
k[MACR+hv-->MACO3+HO2]=CONST(J19)
k[NO3+MACR-->MACO3+HNO3]=CONST(3.4D-15)
k[O3+MACR-->HCHO+MGLYOOB]=CONST(1.4D-15*EXP(-2100/(T))*0.12)
k[O3+MACR-->MGLYOX+CH2OOG]=CONST(1.4D-15*EXP(-2100/(T))*0.88)
k[OH+MACR-->MACO3]=CONST(8.0D-12*EXP(380/(T))*0.45)
k[OH+MACR-->MACRO2]=CONST(8.0D-12*EXP(380/(T))*0.47)
k[OH+MACR-->MACROHO2]=CONST(8.0D-12*EXP(380/(T))*0.08)
k[MVK+hv-->C3H6+CO]=CONST(J23)
k[MVK+hv-->CH3CO3+HCHO+CO+HO2]=CONST(J24)
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k[O3+MVK-->MGLOOA+HCHO]=CONST(8.5D-16*EXP(-1520/(T))*0.5)
k[O3+MVK-->MGLYOX+CH2OOB]=CONST(8.5D-16*EXP(-1520/(T))*0.5)
k[OH+MVK-->HMVKAO2]=CONST(2.6D-12*EXP(610/(T))*0.3)
k[OH+MVK-->HMVKBO2]=CONST(2.6D-12*EXP(610/(T))*0.7)
k[HCHO+hv-->CO+HO2+HO2]=CONST(J11)
k[HCHO+hv-->H2+CO]=CONST(J12)
k[NO3+HCHO-->HNO3+CO+HO2]=CONST(5.5D-16)
k[OH+HCHO-->HO2+CO]=CONST(5.4D-12*EXP(135/(T)))
k[CISOPA-->CISOPAO2]=CONST(3.50D-12*O2)
k[CISOPA-->ISOPBO2]=CONST(3.00D-12*O2)
k[CISOPC-->CISOPCO2]=CONST(2.00D-12*O2)
k[CISOPC-->ISOPDO2]=CONST(3.50D-12*O2)
k[ISOP34O2+HO2-->ISOP34OOH]=CONST(KRO2HO2*0.706)
k[ISOP34O2+NO-->ISOP34NO3]=CONST(KRO2NO*0.087)
k[ISOP34O2+NO-->ISOP34O+NO2]=CONST(KRO2NO*0.913)
k[ISOP34O2+NO3-->ISOP34O+NO2]=CONST(KRO2NO3)
k[ISOP34O2-->HC4CHO]=CONST(2.65D-12*RO2*0.1)
k[ISOP34O2-->ISOP34O]=CONST(2.65D-12*RO2*0.8)
k[ISOP34O2-->ISOPDOH]=CONST(2.65D-12*RO2*0.1)
k[ME3BU3ECHO+NO3-->NC526O2]=CONST(3.30D-13)
k[ME3BU3ECHO+O3-->CH2OOC+CO2C3CHO]=CONST(1.60D-17*0.33)
k[ME3BU3ECHO+O3-->CO2C3OOB+HCHO]=CONST(1.60D-17*0.67)
k[ME3BU3ECHO+OH-->C530O2]=CONST(7.30D-11*0.712)
k[ME3BU3ECHO+OH-->M3BU3ECO3]=CONST(7.30D-11*0.288)
k[ME3BU3ECHO+hv-->C45O2+CO+HO2]=CONST(J15)
k[PE4E2CO+NO3-->NC51O2]=CONST(1.20D-14)
k[PE4E2CO+O3-->CH2OOB+CO2C3CHO]=CONST(1.00D-17*0.43)
k[PE4E2CO+O3-->CO2C3OOA+HCHO]=CONST(1.00D-17*0.57)
k[PE4E2CO+OH-->C51O2]=CONST(2.71D-11)
k[PE4E2CO+hv-->CH3CO3+CH2CHCH2O2]=CONST(J22)
k[TISOPA-->ISOPAO2]=CONST(2.50D-12*EXP(-480/(T))*O2)
k[TISOPA-->ISOPBO2]=CONST(3.00D-12*O2)
k[TISOPC-->ISOPCO2]=CONST(2.50D-12*EXP(-480/(T))*O2)
k[TISOPC-->ISOPDO2]=CONST(3.50D-12*O2)
k[CH3C2H2O2-->CH3CO3+HCHO]=CONST(KDEC*0.35)
k[CH3C2H2O2-->HCHO+CH3O2+CO]=CONST(KDEC*0.65)
k[MACO3+HO2-->CH3C2H2O2+OH]=CONST(KAPHO2*0.44)
k[MACO3+HO2-->MACO2H+O3]=CONST(KAPHO2*0.15)
k[MACO3+HO2-->MACO3H]=CONST(KAPHO2*0.41)
k[MACO3+NO-->CH3C2H2O2+NO2]=CONST(8.70D-12*EXP(290/(T)))
k[MACO3+NO2-->MPAN]=CONST(KFPAN)
k[MACO3+NO3-->CH3C2H2O2+NO2]=CONST(KRO2NO3*1.74)
k[MACO3-->CH3C2H2O2]=CONST(1.00D-11*0.7*RO2)
k[MACO3-->MACO2H]=CONST(1.00D-11*0.3*RO2)
k[MGLYOOB-->MGLYOO]=CONST(KDEC*0.18)
k[MGLYOOB-->OH+CO+CH3CO3]=CONST(KDEC*0.82)
k[MGLYOX+hv-->CH3CO3+CO+HO2]=CONST(J34)
k[NO3+MGLYOX-->CH3CO3+CO+HNO3]=CONST(KNO3AL*2.4)
k[OH+MGLYOX-->CH3CO3+CO]=CONST(1.9D-12*EXP(575/(T)))
k[CH2OOG-->CH2OO]=CONST(KDEC*0.37)
k[CH2OOG-->CO]=CONST(KDEC*0.47)
k[CH2OOG-->HO2+CO+OH]=CONST(KDEC*0.16)
k[MACRO2+HO2-->MACROOH]=CONST(KRO2HO2*0.625)
k[MACRO2+NO-->MACRNO3]=CONST(KRO2NO*0.013)
k[MACRO2+NO-->MACRO+NO2]=CONST(KRO2NO*0.987)
k[MACRO2+NO3-->MACRO+NO2]=CONST(KRO2NO3)
k[MACRO2-->ACETOL+CO+OH]=CONST(K14ISOM1)
k[MACRO2-->MACRO]=CONST(9.20D-14*0.7*RO2)
k[MACRO2-->MACROH]=CONST(9.20D-14*0.3*RO2)
k[MACROHO2+HO2-->MACROHOOH]=CONST(KRO2HO2*0.625)
k[MACROHO2+NO-->MACRNB]=CONST(KRO2NO*0.017)
k[MACROHO2+NO-->MACROHO+NO2]=CONST(KRO2NO*0.983)
k[MACROHO2+NO3-->MACROHO+NO2]=CONST(KRO2NO3)
k[MACROHO2-->C3MDIALOH]=CONST(1.4D-12*0.2*RO2)
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k[MACROHO2-->MACROH]=CONST(1.4D-12*0.2*RO2)
k[MACROHO2-->MACROHO]=CONST(1.4D-12*0.6*RO2)
k[NO3+C3H6-->PRONO3AO2]=CONST(4.6D-13*EXP(-1155/(T))*0.35)
k[NO3+C3H6-->PRONO3BO2]=CONST(4.6D-13*EXP(-1155/(T))*0.65)
k[OH+C3H6-->HYPROPO2]=CONST(KMT16*0.87)
k[OH+C3H6-->IPROPOLO2]=CONST(KMT16*0.13)
k[CH3CO3+HO2-->CH3CO2H+O3]=CONST(KAPHO2*0.15)
k[CH3CO3+HO2-->CH3CO3H]=CONST(KAPHO2*0.41)
k[CH3CO3+HO2-->CH3O2+OH]=CONST(KAPHO2*0.44)
k[CH3CO3+NO-->NO2+CH3O2]=CONST(7.5D-12*EXP(290/(T)))
k[CH3CO3+NO2-->PAN]=CONST(KFPAN)
k[CH3CO3+NO3-->NO2+CH3O2]=CONST(4.0D-12)
k[CH3CO3-->CH3CO2H]=CONST(1.00D-11*0.3*RO2)
k[CH3CO3-->CH3O2]=CONST(1.00D-11*0.7*RO2)
k[MGLOOA-->CH3CHO]=CONST(KDEC*0.20)
k[MGLOOA-->CH3CO3+HCHO+HO2]=CONST(KDEC*0.20)
k[MGLOOA-->MGLOO]=CONST(KDEC*0.24)
k[MGLOOA-->OH+CO+CH3CO3]=CONST(KDEC*0.36)
k[HMVKAO2+HO2-->HMVKAOOH]=CONST(KRO2HO2*0.625)
k[HMVKAO2+NO-->HMVKANO3]=CONST(KRO2NO*0.017)
k[HMVKAO2+NO-->HMVKAO+NO2]=CONST(KRO2NO*0.983)
k[HMVKAO2+NO3-->HMVKAO+NO2]=CONST(KRO2NO3)
k[HMVKAO2-->CO2H3CHO]=CONST(2.00D-12*0.2*RO2)
k[HMVKAO2-->HMVKAO]=CONST(2.00D-12*0.6*RO2)
k[HMVKAO2-->HO12CO3C4]=CONST(2.00D-12*0.2*RO2)
k[HMVKBO2+NO-->MVKNO3]=CONST(KRO2NO*0.043)
k[HMVKBO2+HO2-->HMVKBOOH]=CONST(KRO2HO2*0.625)
k[HMVKBO2+NO-->HMVKBO+NO2]=CONST(KRO2NO*0.957)
k[HMVKBO2+NO3-->HMVKBO+NO2]=CONST(KRO2NO3)
k[HMVKBO2-->BIACETOH]=CONST(8.80D-13*0.2*RO2)
k[HMVKBO2-->HMVKBO]=CONST(8.80D-13*0.6*RO2)
k[HMVKBO2-->HO12CO3C4]=CONST(8.80D-13*0.2*RO2)
k[MACROO+CO-->MACR]=CONST(1.2D-15)
k[MACROO+NO-->MACR+NO2]=CONST(1.0D-14)
k[MACROO+NO2-->MACR+NO3]=CONST(1.0D-15)
k[MACROO+SO2-->MACR+SO3]=CONST(7.0D-14)
k[MACROO-->MACO2H]=CONST(1.0D-17*H2O)
k[MACROO-->MACR+H2O2]=CONST(6.0D-18*H2O)
k[CH3O2+HO2-->CH3OOH]=CONST(3.8D-13*EXP(780/(T))*(1-1/(1+498*EXP(-1160/(T)))))
k[CH3O2+HO2-->HCHO]=CONST(3.8D-13*EXP(780/(T))*(1/(1+498*EXP(-1160/(T)))))
k[CH3O2+NO-->CH3NO3]=CONST(2.3D-12*EXP(360/(T))*0.001)
k[CH3O2+NO-->CH3O+NO2]=CONST(2.3D-12*EXP(360/(T))*0.999)
k[CH3O2+NO2-->CH3O2NO2]=CONST(KMT13)
k[CH3O2+NO3-->CH3O+NO2]=CONST(1.2D-12)
k[CH3O2-->CH3O]=CONST(2*KCH3O2*RO2*7.18*EXP(-885/(T)))
k[CH3O2-->CH3OH]=CONST(2*KCH3O2*RO2*0.5*(1-7.18*EXP(-885/(T))))
k[CH3O2-->HCHO]=CONST(2*KCH3O2*RO2*0.5*(1-7.18*EXP(-885/(T))))
k[MVKOO+CO-->MVK]=CONST(1.2D-15)
k[MVKOO+NO-->MVK+NO2]=CONST(1.0D-14)
k[MVKOO+NO2-->MVK+NO3]=CONST(1.0D-15)
k[MVKOO+SO2-->MVK+SO3]=CONST(7.0D-14)
k[MVKOO-->MVK+H2O2]=CONST(6.0D-18*H2O)
k[MVKO2+HO2-->MVKOOH]=CONST(KRO2HO2*0.625)
k[MVKO2+NO-->MVKO+NO2]=CONST(KRO2NO)
k[MVKO2+NO3-->MVKO+NO2]=CONST(KRO2NO3)
k[MVKO2-->MVKO]=CONST(2.00D-12*0.6*RO2)
k[MVKO2-->MVKOH]=CONST(2.00D-12*0.2*RO2)
k[MVKO2-->VGLYOX]=CONST(2.00D-12*0.2*RO2)
k[CISOPAO2+HO2-->ISOPAOOH]=CONST(KRO2HO2*0.706)
k[CISOPAO2+NO-->CISOPAO+NO2]=CONST(KRO2NO*0.913)
k[CISOPAO2+NO-->ISOPANO3]=CONST(KRO2NO*0.087)
k[CISOPAO2+NO3-->CISOPAO+NO2]=CONST(KRO2NO3)
k[CISOPAO2-->C536O2]=CONST(8.14D9*EXP(-8591/(T))*EXP(1.00D8/(T)@3)*0.5)
k[CISOPAO2-->C5HPALD1+HO2]=CONST(8.14D9*EXP(-8591/(T))*EXP(1.00D8/(T)@3)*0.5)
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k[CISOPAO2-->CISOPA]=CONST(5.22D15*EXP(-9838/(T)))
k[CISOPAO2-->CISOPAO]=CONST(2.40D-12*0.8*RO2)
k[CISOPAO2-->HC4ACHO]=CONST(2.40D-12*0.1*RO2)
k[CISOPAO2-->ISOPAOH]=CONST(2.40D-12*0.1*RO2)
k[ISOPBO2+HO2-->ISOPBOOH]=CONST(KRO2HO2*0.706)
k[ISOPBO2+NO-->ISOPBNO3]=CONST(KRO2NO*0.104)
k[ISOPBO2+NO-->ISOPBO+NO2]=CONST(KRO2NO*0.896)
k[ISOPBO2+NO3-->ISOPBO+NO2]=CONST(KRO2NO3)
k[ISOPBO2-->CISOPA]=CONST(8.62D15*EXP(-11322/(T)))
k[ISOPBO2-->ISOPBO]=CONST(8.00D-13*0.8*RO2)
k[ISOPBO2-->ISOPBOH]=CONST(8.00D-13*0.2*RO2)
k[ISOPBO2-->MVK+HCHO+OH]=CONST(1.04D11*EXP(-9746/(T)))
k[ISOPBO2-->TISOPA]=CONST(8.55D15*EXP(-10743/(T)))
k[CISOPCO2+HO2-->ISOPCOOH]=CONST(KRO2HO2*0.706)
k[CISOPCO2+NO-->CISOPCO+NO2]=CONST(KRO2NO*0.913)
k[CISOPCO2+NO-->ISOPCNO3]=CONST(KRO2NO*0.087)
k[CISOPCO2+NO3-->CISOPCO+NO2]=CONST(KRO2NO3)
k[CISOPCO2-->C537O2]=CONST(2.20D10*EXP(-8174/(T))*EXP(1.00D8/(T)@3)*0.5)
k[CISOPCO2-->C5HPALD2+HO2]=CONST(2.20D10*EXP(-8174/(T))*EXP(1.00D8/(T)@3)*0.5)
k[CISOPCO2-->CISOPC]=CONST(3.06D15*EXP(-10254/(T)))
k[CISOPCO2-->CISOPCO]=CONST(2.00D-12*0.8*RO2)
k[CISOPCO2-->HC4CCHO]=CONST(2.00D-12*0.1*RO2)
k[CISOPCO2-->ISOPAOH]=CONST(2.00D-12*0.1*RO2)
k[ISOPDO2+HO2-->ISOPDOOH]=CONST(KRO2HO2*0.706)
k[ISOPDO2+NO-->ISOPDNO3]=CONST(KRO2NO*0.104)
k[ISOPDO2+NO-->ISOPDO+NO2]=CONST(KRO2NO*0.896)
k[ISOPDO2+NO3-->ISOPDO+NO2]=CONST(KRO2NO3)
k[ISOPDO2-->CISOPC]=CONST(1.05D16*EXP(-11705/(T)))
k[ISOPDO2-->HCOC5]=CONST(2.90D-12*0.1*RO2)
k[ISOPDO2-->ISOPDO]=CONST(2.90D-12*0.8*RO2)
k[ISOPDO2-->ISOPDOH]=CONST(2.90D-12*0.1*RO2)
k[ISOPDO2-->MACR+HCHO+OH]=CONST(1.88D11*EXP(-9752/(T)))
k[ISOPDO2-->TISOPC]=CONST(1.05D16*EXP(-11569/(T)))
k[ISOP34OOH+OH-->HC4CHO+OH]=CONST(9.73D-11)
k[ISOP34OOH+hv-->ISOP34O+OH]=CONST(J41)
k[ISOP34NO3+OH-->INAO2]=CONST(8.77D-11)
k[O3+ISOP34NO3-->HMVKANO3+CH2OOC]=CONST(2.52D-17*0.50)
k[O3+ISOP34NO3-->NC41OOA+HCHO]=CONST(2.52D-17*0.50)
k[ISOP34O-->MACR+HCHO+HO2]=CONST(KDEC)
k[HC4CHO+OH-->C58O2]=CONST(1.04D-10*0.829)
k[HC4CHO+OH-->HC4CO3]=CONST(1.04D-10*0.171)
k[HC4CHO+hv-->MACR+CO+HO2+HO2]=CONST(J15)
k[OH+ISOPDOH-->HCOC5+HO2]=CONST(7.38D-11)
k[NC526O2+HO2-->NC526OOH]=CONST(KRO2HO2*0.706)
k[NC526O2+NO-->NC526O+NO2]=CONST(KRO2NO)
k[NC526O2+NO3-->NC526O+NO2]=CONST(KRO2NO3)
k[NC526O2-->NC526O]=CONST(9.20D-14*RO2)
k[CH2OOC-->CH2OO]=CONST(KDEC*0.18)
k[CH2OOC-->HO2+CO+OH]=CONST(KDEC*0.82)
k[CO2C3CHO+NO3-->CO2C3CO3+HNO3]=CONST(KNO3AL*4.0)
k[CO2C3CHO+OH-->CO2C3CO3]=CONST(7.15D-11)
k[CO2C3CHO+hv-->CH3COCH2O2+HCHO]=CONST(J15)
k[CO2C3OOB-->C4CO2O2+OH]=CONST(KDEC*0.82)
k[CO2C3OOB-->CO2C3OO]=CONST(KDEC*0.18)
k[C530O2+HO2-->C530OOH]=CONST(KRO2HO2*0.706)
k[C530O2+NO-->C530NO3]=CONST(KRO2NO*0.020)
k[C530O2+NO-->C530O+NO2]=CONST(KRO2NO*0.980)
k[C530O2+NO3-->C530O+NO2]=CONST(KRO2NO3)
k[C530O2-->C530O]=CONST(9.20D-14*RO2)
k[M3BU3ECO3+HO2-->C45O2+OH+NO2]=CONST(KAPHO2*0.44)
k[M3BU3ECO3+HO2-->M3BU3ECO3H]=CONST(KAPHO2*0.56)
k[M3BU3ECO3+NO-->C45O2+NO2]=CONST(KAPNO)
k[M3BU3ECO3+NO2-->M3BU3EPAN]=CONST(KFPAN)
k[M3BU3ECO3+NO3-->C45O2+NO2]=CONST(KRO2NO3*1.6)
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k[M3BU3ECO3-->C45O2]=CONST(1.00D-11*RO2)
k[C45O2+HO2-->C45OOH]=CONST(KRO2HO2*0.625)
k[C45O2+NO-->C45NO3]=CONST(KRO2NO*0.024)
k[C45O2+NO-->C45O+NO2]=CONST(KRO2NO*0.976)
k[C45O2+NO3-->C45O+NO2]=CONST(KRO2NO3)
k[C45O2-->C45O]=CONST(1.30D-12*RO2)
k[NC51O2+HO2-->NC51OOH]=CONST(KRO2HO2*0.706)
k[NC51O2+NO-->NC51O+NO2]=CONST(KRO2NO)
k[NC51O2+NO3-->NC51O+NO2]=CONST(KRO2NO3)
k[NC51O2-->NC51O]=CONST(8.80D-13*RO2)
k[CO2C3OOA-->C4CO2O2+OH]=CONST(KDEC*0.36)
k[CO2C3OOA-->CH3COCH2O2+HO2]=CONST(KDEC*0.2)
k[CO2C3OOA-->CH3COCH3]=CONST(KDEC*0.2)
k[CO2C3OOA-->CO2C3OO]=CONST(KDEC*0.24)
k[C51O2+HO2-->C51OOH]=CONST(KRO2HO2*0.706)
k[C51O2+NO-->C51NO3]=CONST(KRO2NO*0.065)
k[C51O2+NO-->C51O+NO2]=CONST(KRO2NO*0.935)
k[C51O2+NO3-->C51O+NO2]=CONST(KRO2NO3)
k[C51O2-->C51O]=CONST(8.40D-13*0.6*RO2)
k[C51O2-->C51OH]=CONST(8.40D-13*0.2*RO2)
k[C51O2-->HO1CO24C5]=CONST(8.40D-13*0.2*RO2)
k[CH2CHCH2O2+HO2-->CH2CHCH2OOH]=CONST(KRO2HO2*0.520)
k[CH2CHCH2O2+NO-->CH2CHCH2NO3]=CONST(KRO2NO*0.024)
k[CH2CHCH2O2+NO-->CH2CHCH2O+NO2]=CONST(KRO2NO*0.976)
k[CH2CHCH2O2+NO3-->CH2CHCH2O+NO2]=CONST(KRO2NO3)
k[CH2CHCH2O2-->ACR]=CONST(1.30D-12*0.2*RO2)
k[CH2CHCH2O2-->ALLYLOH]=CONST(1.30D-12*0.2*RO2)
k[CH2CHCH2O2-->CH2CHCH2O]=CONST(1.30D-12*0.6*RO2)
k[ISOPAO2+HO2-->ISOPAOOH]=CONST(KRO2HO2*0.706)
k[ISOPAO2+NO-->ISOPANO3]=CONST(KRO2NO*0.087)
k[ISOPAO2+NO-->ISOPAO+NO2]=CONST(KRO2NO*0.913)
k[ISOPAO2+NO3-->ISOPAO+NO2]=CONST(KRO2NO3)
k[ISOPAO2-->HC4ACHO]=CONST(2.40D-12*0.1*RO2)
k[ISOPAO2-->ISOPAO]=CONST(2.40D-12*0.8*RO2)
k[ISOPAO2-->ISOPAOH]=CONST(2.40D-12*0.1*RO2)
k[ISOPAO2-->TISOPA]=CONST(2.86D14*EXP(-9028/(T)))
k[ISOPCO2+HO2-->ISOPCOOH]=CONST(KRO2HO2*0.706)
k[ISOPCO2+NO-->CISOPCO+NO2]=CONST(KRO2NO*0.913)
k[ISOPCO2+NO-->ISOPCNO3]=CONST(KRO2NO*0.087)
k[ISOPCO2+NO3-->CISOPCO+NO2]=CONST(KRO2NO3)
k[ISOPCO2-->CISOPCO]=CONST(2.00D-12*0.8*RO2)
k[ISOPCO2-->HC4CCHO]=CONST(2.00D-12*0.1*RO2)
k[ISOPCO2-->ISOPAOH]=CONST(2.00D-12*0.1*RO2)
k[ISOPCO2-->TISOPC]=CONST(2.13D14*EXP(-9984/(T)))
k[HCOOH+OH-->HO2]=CONST(4.5D-13)
k[OH+MACO2H-->CH3C2H2O2]=CONST(1.51D-11)
k[MACO3H+hv-->CH3C2H2O2+OH]=CONST(J41)
k[OH+MACO3H-->ACETOL+CO+OH]=CONST(1.30D-11*0.83)
k[OH+MACO3H-->HMML+OH]=CONST(1.30D-11*0.17)
k[OH+MACO3H-->MACO3]=CONST(3.60D-12)
k[MPAN-->MACO3+NO2]=CONST(1.6D+16*EXP(-13500/(T)))
k[O3+MPAN-->HCHO+CH3CO3+NO3]=CONST(8.2D-18)
k[OH+MPAN-->ACETOL+CO+NO3]=CONST(2.9D-11*0.22)
k[OH+MPAN-->HMML+NO3]=CONST(2.90D-11*0.57)
k[OH+MPAN-->MAE+NO3]=CONST(2.90D-11*0.21)
k[MGLYOO+CO-->MGLYOX]=CONST(1.2D-15)
k[MGLYOO+NO-->MGLYOX+NO2]=CONST(1.0D-14)
k[MGLYOO+NO2-->MGLYOX+NO3]=CONST(1.0D-15)
k[MGLYOO+SO2-->MGLYOX+SO3]=CONST(7.0D-14)
k[MGLYOO-->MGLYOX+H2O2]=CONST(6.0D-18*H2O)
k[MACROOH+hv-->ACETOL+CO+HO2+OH]=CONST(J17)
k[MACROOH+hv-->MACRO+OH]=CONST(J41)
k[OH+MACROOH-->ACETOL+CO+OH]=CONST(3.77D-11)
k[MACRNO3+OH-->CONM2CHO+HO2]=CONST(4.34D-12*0.16)
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k[MACRNO3+OH-->MACRNCO3]=CONST(4.34D-12*0.84)
k[MACRNO3+hv-->ACETOL+NO2+CO+HO2]=CONST(J56*10)
k[MACRO-->ACETOL+CO+HO2]=CONST(KDEC)
k[ACETOL+OH-->MGLYOX+HO2]=CONST(1.6D-12*EXP(305/(T)))
k[ACETOL+hv-->CH3CO3+HCHO+HO2]=CONST(J22)
k[MACROH+hv-->ACETOL+CO+HO2+HO2]=CONST(J17)
k[OH+MACROH-->C3MDIALOH+HO2]=CONST(3.42D-11)
k[MACROHOOH+OH-->C3MDIALOH+OH]=CONST(5.55D-11)
k[MACROHOOH+hv-->IBUTALOH+CO+HO2+OH]=CONST(J17)
k[MACROHOOH+hv-->MACROHO+OH]=CONST(J41)
k[MACRNB+hv-->C3MDIALOH+HO2+NO2]=CONST(J56*1.6)
k[OH+MACRNB-->MACRNBCO3]=CONST(2.15D-11)
k[MACROHO-->MGLYOX+HCHO+HO2]=CONST(KDEC)
k[C3MDIALOH+OH-->CHOMOHCO3]=CONST(4.18D-11)
k[C3MDIALOH+hv-->MGLYOX+HO2+CO+HO2]=CONST(J17*2)
k[PRONO3AO2+NO-->PRONO3AO+NO2]=CONST(KRO2NO)
k[PRONO3AO2+NO3-->PRONO3AO+NO2]=CONST(KRO2NO3)
k[PRONO3AO2-->CHOPRNO3]=CONST(6.00D-13*0.2*RO2)
k[PRONO3AO2-->PRONO3AO]=CONST(6.00D-13*0.6*RO2)
k[PRONO3AO2-->PROPOLNO3]=CONST(6.00D-13*0.2*RO2)
k[PRONO3BO2+NO-->PRONO3BO+NO2]=CONST(KRO2NO)
k[PRONO3BO2+NO3-->PRONO3BO+NO2]=CONST(KRO2NO3)
k[PRONO3BO2-->NOA]=CONST(4.00D-14*0.2*RO2)
k[PRONO3BO2-->PROLNO3]=CONST(4.00D-14*0.2*RO2)
k[PRONO3BO2-->PRONO3BO]=CONST(4.00D-14*0.6*RO2)
k[CH3CHO+hv-->CH3O2+HO2+CO]=CONST(J13)
k[NO3+CH3CHO-->HNO3+CH3CO3]=CONST(1.4D-12*EXP(-1860/(T)))
k[OH+CH3CHO-->CH3CO3]=CONST(4.7D-12*EXP(345/(T))*0.95)
k[OH+CH3CHO-->HCOCH2O2]=CONST(4.7D-12*EXP(345/(T))*0.05)
k[HYPROPO2+HO2-->HYPROPO2H]=CONST(KRO2HO2*0.520)
k[HYPROPO2+NO3-->HYPROPO+NO2]=CONST(KRO2NO3)
k[HYPROPO2-->ACETOL]=CONST(8.80D-13*0.2*RO2)
k[HYPROPO2-->HYPROPO]=CONST(8.80D-13*0.6*RO2)
k[HYPROPO2-->PROPGLY]=CONST(8.80D-13*0.2*RO2)
k[NO+HYPROPO2-->HYPROPO+NO2]=CONST(KRO2NO*0.977)
k[NO+HYPROPO2-->PROPOLNO3]=CONST(KRO2NO*0.023)
k[IPROPOLO2+HO2-->IPROPOLO2H]=CONST(KRO2HO2*0.520)
k[IPROPOLO2+NO-->IPROPOLO+NO2]=CONST(KRO2NO*0.991)
k[IPROPOLO2+NO-->PROLNO3]=CONST(KRO2NO*0.009)
k[IPROPOLO2+NO3-->IPROPOLO+NO2]=CONST(KRO2NO3)
k[IPROPOLO2-->CH3CHOHCHO]=CONST(2.00D-12*0.2*RO2)
k[IPROPOLO2-->IPROPOLO]=CONST(2.00D-12*0.6*RO2)
k[IPROPOLO2-->PROPGLY]=CONST(2.00D-12*0.2*RO2)
k[CH3CO2H+OH-->CH3O2]=CONST(8.00D-13)
k[CH3CO3H+OH-->CH3CO3]=CONST(3.70D-12)
k[CH3CO3H+hv-->CH3O2+OH]=CONST(J41)
k[PAN+OH-->HCHO+CO+NO2]=CONST(3D-14)
k[PAN-->CH3CO3+NO2]=CONST(KBPAN)
k[MGLOO+CO-->MGLYOX]=CONST(1.2D-15)
k[MGLOO+NO-->MGLYOX+NO2]=CONST(1.0D-14)
k[MGLOO+NO2-->MGLYOX+NO3]=CONST(1.0D-15)
k[MGLOO+SO2-->MGLYOX+SO3]=CONST(7.0D-14)
k[MGLOO-->CH3COCO2H]=CONST(1.0D-17*H2O)
k[MGLOO-->MGLYOX+H2O2]=CONST(6.0D-18*H2O)
k[HMVKAOOH+hv-->HMVKAO+OH]=CONST(J41)
k[OH+HMVKAOOH-->CO2H3CHO+OH]=CONST(5.77D-11)
k[HMVKANO3+hv-->HMVKAO+NO2]=CONST(J56*0.91)
k[OH+HMVKANO3-->CO2H3CHO+NO2]=CONST(2.23D-12)
k[HMVKAO-->MGLYOX+HCHO+HO2]=CONST(KDEC)
k[CO2H3CHO+hv-->MGLYOX+CO+HO2+HO2]=CONST(J15)
k[NO3+CO2H3CHO-->CO2H3CO3+HNO3]=CONST(KNO3AL*4.0)
k[OH+CO2H3CHO-->CO2H3CO3]=CONST(2.45D-11)
k[HO12CO3C4+hv-->CH3CO3+HOCH2CHO+HO2]=CONST(J22)
k[OH+HO12CO3C4-->BIACETOH+HO2]=CONST(1.88D-11)
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k[MVKNO3+OH-->BIACETOH+NO2]=CONST(1.33D-12*0.33)
k[MVKNO3+OH-->CO2N3CHO+HO2]=CONST(1.33D-12*0.67)
k[MVKNO3+hv-->CH3CO3+HOCH2CHO+NO2]=CONST(J56*1.6)
k[HMVKBOOH+hv-->HMVKBO+OH]=CONST(J41)
k[OH+HMVKBOOH-->BIACETOH+OH]=CONST(3.95D-11)
k[HMVKBO-->CH3CO3+HOCH2CHO]=CONST(KDEC)
k[BIACETOH+hv-->CH3CO3+HOCH2CO3]=CONST(J35)
k[OH+BIACETOH-->CO23C3CHO+HO2]=CONST(2.69D-12)
k[CH3OOH+hv-->CH3O+OH]=CONST(J41)
k[OH+CH3OOH-->CH3O2]=CONST(5.3D-12*EXP(190/(T))*0.6)
k[OH+CH3OOH-->HCHO+OH]=CONST(5.3D-12*EXP(190/(T))*0.4)
k[CH3NO3+hv-->CH3O+NO2]=CONST(J51)
k[OH+CH3NO3-->HCHO+NO2]=CONST(4.0D-13*EXP(-845/(T)))
k[CH3O-->HCHO+HO2]=CONST(7.2D-14*EXP(-1080/(T))*O2)
k[CH3O2NO2-->CH3O2+NO2]=CONST(KMT14)
k[CH3OH+OH-->HO2+HCHO]=CONST(2.85D-12*EXP(-345/(T)))
k[MVKOOH+hv-->HCHO+OH+ACO3]=CONST(J24)
k[MVKOOH+hv-->MVKO+OH]=CONST(J41)
k[OH+MVKOOH-->MVKO2]=CONST(1.90D-12*EXP(190/(T)))
k[OH+MVKOOH-->VGLYOX+OH]=CONST(2.55D-11)
k[MVKO-->HCHO+ACO3]=CONST(KDEC)
k[MVKOH+O3-->HMGLOOA+HCHO]=CONST(7.51D-16*EXP(-1521/(T))*0.5)
k[MVKOH+O3-->HOCH2COCHO+CH2OOB]=CONST(7.51D-16*EXP(-1521/(T))*0.5)
k[MVKOH+OH-->MVKOHAO2]=CONST(4.60D-12*EXP(452/(T))*0.3)
k[MVKOH+OH-->MVKOHBO2]=CONST(4.60D-12*EXP(452/(T))*0.7)
k[MVKOH+hv-->ALLYLOH+CO]=CONST(J23)
k[MVKOH+hv-->HCHO+HO2+HOCH2CO3+CO]=CONST(J24)
k[NO3+VGLYOX-->CO+ACO3+HNO3]=CONST(KNO3AL*2.0)
k[OH+VGLYOX-->CO+ACO3]=CONST(2.95D-11)
k[VGLYOX+hv-->HO2+CO+ACO3]=CONST(J34)
k[ISOPAOOH+hv-->ISOPAO+OH]=CONST(J41)
k[OH+ISOPAOOH-->HC4ACHO+OH]=CONST(1.54D-10*0.05)
k[OH+ISOPAOOH-->IEPOXA+OH]=CONST(1.54D-10*0.93)
k[OH+ISOPAOOH-->ISOPAO2]=CONST(1.54D-10*0.02)
k[CISOPAO-->C526O2]=CONST(KDEC*0.19)
k[CISOPAO-->HC4CCHO+HO2]=CONST(KDEC*0.63)
k[CISOPAO-->M3F+HO2]=CONST(KDEC*0.18)
k[ISOPANO3+hv-->ISOPAO+NO2]=CONST(J53)
k[O3+ISOPANO3-->ACETOL+NC2OOA]=CONST(4.10D-17*0.50)
k[O3+ISOPANO3-->ACLOOA+NO3CH2CHO]=CONST(4.10D-17*0.50)
k[OH+ISOPANO3-->INAO2]=CONST(1.12D-10)
k[C536O2+HO2-->C536OOH]=CONST(KRO2HO2*0.706)
k[C536O2+NO-->C536O+NO2]=CONST(KRO2NO)
k[C536O2+NO3-->C536O+NO2]=CONST(KRO2NO3)
k[C536O2-->C536O]=CONST(9.20D-14*RO2)
k[C536O2-->DHPMEK+CO+OH]=CONST(K14ISOM1)
k[C5HPALD1+NO3-->C5PACALD1+OH+HNO3]=CONST(KNO3AL*4.25)
k[C5HPALD1+O3-->MGLYOOA+HCOCH2OOH]=CONST(2.40D-17*0.73)
k[C5HPALD1+O3-->MGLYOX+PGAOOB]=CONST(2.40D-17*0.27)
k[C5HPALD1+OH-->C4MALOHOOH+OH]=CONST(5.20D-11*0.359)
k[C5HPALD1+OH-->C4MDIAL+OH]=CONST(5.20D-11*0.256)
k[C5HPALD1+OH-->C5PACALD1+OH]=CONST(5.20D-11*0.385)
k[C5HPALD1+hv-->CH3CO3+HOCH2CHO+CO+OH]=CONST(J20*0.5)
k[C5HPALD1+hv-->HVMK+CO+OH+OH]=CONST(J20*0.5)
k[HC4ACHO+hv-->ACETOL+HO2+HO2+CO+CO]=CONST(J18)
k[HC4ACHO+hv-->HC4ACO3+HO2]=CONST(J19)
k[NO3+HC4ACHO-->HC4ACO3+HNO3]=CONST(KNO3AL*4.25)
k[O3+HC4ACHO-->ACETOL+GLYOOC]=CONST(2.40D-17*0.5)
k[O3+HC4ACHO-->ACLOOA+GLYOX]=CONST(2.40D-17*0.5)
k[OH+HC4ACHO-->C4MDIAL+HO2]=CONST(6.42D-11*0.051)
k[OH+HC4ACHO-->C58AO2]=CONST(6.42D-11*0.247)
k[OH+HC4ACHO-->C58O2]=CONST(6.42D-11*0.452)
k[OH+HC4ACHO-->HC4ACO3]=CONST(6.42D-11*0.250)
k[OH+ISOPAOH-->HC4ACHO+HO2]=CONST(9.30D-11*0.5)
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k[OH+ISOPAOH-->HC4CCHO+HO2]=CONST(9.30D-11*0.5)
k[ISOPBOOH+hv-->ISOPBO+OH]=CONST(J41)
k[OH+ISOPBOOH-->IEPOXB+OH]=CONST(5.00D-11*0.92)
k[OH+ISOPBOOH-->ISOPBO2]=CONST(5.00D-11*0.08)
k[ISOPBNO3+hv-->ISOPBO+NO2]=CONST(J55)
k[O3+ISOPBNO3-->HCHO+MACRNOOA]=CONST(5.00D-19*0.50)
k[O3+ISOPBNO3-->MACRNO3+CH2OOB]=CONST(5.00D-19*0.50)
k[OH+ISOPBNO3-->INB1O2]=CONST(2.17D-11*0.84)
k[OH+ISOPBNO3-->INB2O2]=CONST(2.17D-11*0.16)
k[ISOPBO-->MVK+HCHO+HO2]=CONST(KDEC)
k[OH+ISOPBOH-->ISOPBO]=CONST(3.85D-11)
k[ISOPCOOH+hv-->CISOPCO+OH]=CONST(J41)
k[OH+ISOPCOOH-->HC4CCHO+OH]=CONST(1.54D-10*0.05)
k[OH+ISOPCOOH-->IEPOXC+OH]=CONST(1.54D-10*0.93)
k[OH+ISOPCOOH-->ISOPCO2]=CONST(1.54D-10*0.02)
k[CISOPCO-->C527O2]=CONST(KDEC*0.30)
k[CISOPCO-->HC4ACHO+HO2]=CONST(KDEC*0.52)
k[CISOPCO-->M3F+HO2]=CONST(KDEC*0.18)
k[ISOPCNO3+hv-->CISOPCO+NO2]=CONST(J53)
k[O3+ISOPCNO3-->GAOOB+NOA]=CONST(4.10D-17*0.50)
k[O3+ISOPCNO3-->HOCH2CHO+NC3OOA]=CONST(4.10D-17*0.50)
k[OH+ISOPCNO3-->INCO2]=CONST(1.12D-10)
k[C537O2+HO2-->C537OOH]=CONST(KRO2HO2*0.706)
k[C537O2+NO-->C537O+NO2]=CONST(KRO2NO)
k[C537O2+NO3-->C537O+NO2]=CONST(KRO2NO3)
k[C537O2-->C537O]=CONST(8.80D-13*RO2)
k[C537O2-->DHPMPAL+CO+OH]=CONST(K14ISOM1)
k[C5HPALD2+NO3-->C5PACALD2+OH+HNO3]=CONST(KNO3AL*4.25)
k[C5HPALD2+O3-->HYPERACET+GLYOOC]=CONST(2.40D-17*0.27)
k[C5HPALD2+O3-->PACLOOA+GLYOX]=CONST(2.40D-17*0.73)
k[C5HPALD2+OH-->C4MDIAL+OH]=CONST(5.20D-11*0.256)
k[C5HPALD2+OH-->C5PACALD2+OH]=CONST(5.20D-11*0.385)
k[C5HPALD2+OH-->HPC52O2]=CONST(5.20D-11*0.359)
k[C5HPALD2+hv-->ACETOL+CO+CO+HO2+OH]=CONST(J20*0.5)
k[C5HPALD2+hv-->HMAC+CO+OH+OH]=CONST(J20*0.5)
k[HC4CCHO+hv-->CH3CO3+HO2+CO+HOCH2CHO]=CONST(J18)
k[HC4CCHO+hv-->HC4CCO3+HO2]=CONST(J19)
k[NO3+HC4CCHO-->HC4CCO3+HNO3]=CONST(KNO3AL*4.25)
k[O3+HC4CCHO-->MGLYOOA+HOCH2CHO]=CONST(2.40D-17*0.5)
k[O3+HC4CCHO-->MGLYOX+GAOOB]=CONST(2.40D-17*0.5)
k[OH+HC4CCHO-->C4MDIAL+HO2]=CONST(6.42D-11*0.051)
k[OH+HC4CCHO-->C57AO2]=CONST(6.42D-11*0.247)
k[OH+HC4CCHO-->C57O2]=CONST(6.42D-11*0.452)
k[OH+HC4CCHO-->HC4CCO3]=CONST(6.42D-11*0.250)
k[ISOPDOOH+hv-->ISOPDO+OH]=CONST(J41)
k[OH+ISOPDOOH-->HCOC5+OH]=CONST(1.15D-10*0.22)
k[OH+ISOPDOOH-->IEPOXB+OH]=CONST(1.15D-10*0.75)
k[OH+ISOPDOOH-->ISOPDO2]=CONST(1.15D-10*0.03)
k[ISOPDNO3+hv-->ISOPDO+NO2]=CONST(J54)
k[O3+ISOPDNO3-->CH2OOC+MVKNO3]=CONST(7.00D-19*0.50)
k[O3+ISOPDNO3-->HCHO+NC4OOA]=CONST(7.00D-19*0.50)
k[OH+ISOPDNO3-->INDO2]=CONST(4.15D-11)
k[ISOPDO-->MACR+HCHO+HO2]=CONST(KDEC)
k[HCOC5+hv-->CH3CO3+HCHO+HOCH2CO3]=CONST(J24)
k[OH+HCOC5-->C59O2]=CONST(3.81D-11)
k[INAO2+HO2-->INAOOH]=CONST(KRO2HO2*0.706)
k[INAO2+NO-->INANO3]=CONST(KRO2NO*0.104)
k[INAO2+NO-->INAO+NO2]=CONST(KRO2NO*0.896)
k[INAO2+NO3-->INAO+NO2]=CONST(KRO2NO3)
k[INAO2-->INAO]=CONST(8.00D-13*0.8*RO2)
k[INAO2-->INAOH]=CONST(8.00D-13*0.2*RO2)
k[NC41OOA-->CO23C4NO3+HO2+OH]=CONST(KDEC*0.82)
k[NC41OOA-->NC41OO]=CONST(KDEC*0.18)
k[C58O2+HO2-->C58OOH]=CONST(KRO2HO2*0.706)
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k[C58O2+NO-->C58NO3]=CONST(KRO2NO*0.019)
k[C58O2+NO-->C58O+NO2]=CONST(KRO2NO*0.981)
k[C58O2+NO3-->C58O+NO2]=CONST(KRO2NO3)
k[C58O2-->C58O]=CONST(9.20D-14*0.7*RO2)
k[C58O2-->C58OH]=CONST(9.20D-14*0.3*RO2)
k[HC4CO3+HO2-->HC4CO3H]=CONST(KAPHO2*0.56)
k[HC4CO3+HO2-->MACR+HO2+OH]=CONST(KAPHO2*0.44)
k[HC4CO3+NO-->MACR+HO2+NO2]=CONST(KAPNO)
k[HC4CO3+NO2-->HC4PAN]=CONST(KFPAN)
k[HC4CO3+NO3-->MACR+HO2+NO2]=CONST(KRO2NO3*1.6)
k[HC4CO3-->MACR+HO2]=CONST(1.00D-11*RO2)
k[NC526OOH+OH-->NC526O2]=CONST(2.22D-11)
k[NC526OOH+hv-->NC526O+OH]=CONST(J41)
k[NC526OOH+hv-->NC526O+OH]=CONST(J15)
k[NC526O-->CO2C3CHO+HCHO+NO2]=CONST(KDEC*0.27)
k[NC526O-->NOA+HCOCH2O2]=CONST(KDEC*0.73)
k[CO2C3CO3+HO2-->CH3COCH2O2+OH]=CONST(KAPHO2*0.44)
k[CO2C3CO3+HO2-->CO2C3CO3H]=CONST(KAPHO2*0.56)
k[CO2C3CO3+NO-->CH3COCH2O2+NO2]=CONST(KAPNO)
k[CO2C3CO3+NO2-->CO2C3PAN]=CONST(KFPAN)
k[CO2C3CO3+NO3-->CH3COCH2O2+NO2]=CONST(KRO2NO3*1.74)
k[CO2C3CO3-->CH3COCH2O2]=CONST(1.00D-11*RO2)
k[CH3COCH2O2+HO2-->CH3COCH2O+OH]=CONST(1.36D-13*EXP(1250/(T))*0.15)
k[CH3COCH2O2+HO2-->HYPERACET]=CONST(1.36D-13*EXP(1250/(T))*0.85)
k[CH3COCH2O2+NO-->CH3COCH2O+NO2]=CONST(KRO2NO)
k[CH3COCH2O2+NO3-->CH3COCH2O+NO2]=CONST(KRO2NO3)
k[CH3COCH2O2-->ACETOL]=CONST(2*(K298CH3O2*8.0D-12)@0.5*RO2*0.2)
k[CH3COCH2O2-->CH3COCH2O]=CONST(2*(K298CH3O2*8.0D-12)@0.5*RO2*0.6)
k[CH3COCH2O2-->MGLYOX]=CONST(2*(K298CH3O2*8.0D-12)@0.5*RO2*0.2)
k[C4CO2O2+HO2-->C4CO2OOH]=CONST(KRO2HO2*0.625)
k[C4CO2O2+NO-->C4CO2O+NO2]=CONST(KRO2NO)
k[C4CO2O2+NO3-->C4CO2O+NO2]=CONST(KRO2NO3)
k[C4CO2O2-->C4CO2O]=CONST(8.80D-12*RO2)
k[CO2C3OO+CO-->CO2C3CHO]=CONST(1.20D-15)
k[CO2C3OO+NO-->CO2C3CHO+NO2]=CONST(1.00D-14)
k[CO2C3OO+NO2-->CO2C3CHO+NO3]=CONST(1.00D-15)
k[CO2C3OO+SO2-->CO2C3CHO+SO3]=CONST(7.00D-14)
k[CO2C3OO-->CO2C3CHO+H2O2]=CONST(6.00D-18*H2O)
k[CO2C3OO-->CO2C3CO2H]=CONST(1.00D-17*H2O)
k[C530OOH+OH-->C530O2]=CONST(2.55D-11)
k[C530OOH+hv-->C530O+OH]=CONST(J41)
k[C530OOH+hv-->C530O+OH]=CONST(J15)
k[C530NO3+OH-->CO2C3CHO+HCHO+NO2]=CONST(1.81D-11)
k[C530NO3+hv-->C530O+NO2]=CONST(J56*4)
k[C530O-->CO2C3CHO+HCHO+HO2]=CONST(KDEC)
k[M3BU3ECO3H+OH-->M3BU3ECO3]=CONST(5.56D-11)
k[M3BU3ECO3H+hv-->C45O2+OH]=CONST(J41)
k[M3BU3EPAN+OH-->MACR+CO+NO2]=CONST(5.20D-11)
k[M3BU3EPAN-->M3BU3ECO3+NO2]=CONST(KBPAN)
k[C45OOH+OH-->MACR+OH]=CONST(6.30D-11)
k[C45OOH+hv-->C45O+OH]=CONST(J41)
k[C45NO3+OH-->MACR+NO2]=CONST(2.47D-11)
k[C45NO3+hv-->C45O+NO2]=CONST(J53)
k[C45O-->MACR+HO2]=CONST(KROPRIM*O2)
k[NC51OOH+OH-->NC51O2]=CONST(8.98D-12)
k[NC51OOH+hv-->NC51O+OH]=CONST(J41)
k[NC51OOH+hv-->NC51O+OH]=CONST(J22)
k[NC51O-->CO2C3CHO+HCHO+NO2]=CONST(KDEC)
k[CH3COCH3+OH-->CH3COCH2O2]=CONST(8.8D-12*EXP(-1320/(T))+1.7D-14*EXP(423/(T)))
k[CH3COCH3+hv-->CH3CO3+CH3O2]=CONST(J21)
k[C51OOH+hv-->C51O+OH]=CONST(J41)
k[C51OOH+hv-->C51O+OH]=CONST(J22)
k[OH+C51OOH-->HO1CO24C5+OH]=CONST(8.69D-11)
k[C51NO3+hv-->C51O+NO2]=CONST(J22)
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k[OH+C51NO3-->HO1CO24C5+NO2]=CONST(1.55D-12)
k[C51O-->CO2C3CHO+HCHO+HO2]=CONST(2.00D+14*EXP(-6382/(T)))
k[OH+C51OH-->HO1CO24C5+OH]=CONST(3.78D-11)
k[HO1CO24C5+hv-->CH3COCH2O2+HOCH2CO3]=CONST(J22*2)
k[OH+HO1CO24C5-->CO24C4CHO+HO2]=CONST(3.22D-12)
k[CH2CHCH2OOH+OH-->ACR+OH]=CONST(5.35D-11)
k[CH2CHCH2OOH+hv-->CH2CHCH2O+OH]=CONST(J41)
k[CH2CHCH2NO3+OH-->ACR+NO2]=CONST(1.28D-11)
k[CH2CHCH2NO3+hv-->CH2CHCH2O+NO2]=CONST(J53)
k[CH2CHCH2O-->ACR+HO2]=CONST(KROPRIM*O2)
k[ACR+NO3-->ACO3+HNO3]=CONST(1.72D-13*EXP(-1190/(T)))
k[ACR+OH-->ACO3]=CONST(0.68*2.00E-11)
k[ACR+OH-->ACRO2]=CONST(0.255*2.00E-11)
k[ACR+OH-->OCCOHCO2]=CONST(0.065*2.00E-11)
k[ACR-->ACO3]=CONST(0.3*J_18)
k[ACR-->C2H4+CO]=CONST(0.4*J_18)
k[ACR-->HCHO+HO2+CO]=CONST(0.3*J_18)
k[O3+ACR-->CH2OOB+GLYOX]=CONST(0.5*2.9E-19)
k[O3+ACR-->GLYOOB+HCHO]=CONST(0.5*2.9E-19)
k[OH+ALLYLOH-->ACR+HO2]=CONST(2.59D-11)
k[ISOPAO-->C524O2]=CONST(KDEC)
k[OH+HMML-->CH3CO3+HCOOH]=CONST(4.33D-12*0.3)
k[OH+HMML-->MGLYOX+OH]=CONST(4.33D-12*0.7)
k[OH+MAE-->CH3COCH2O2]=CONST(8.83D-13)
k[CONM2CHO+OH-->CONM2CO3]=CONST(6.78D-12)
k[CONM2CHO+hv-->MGLYOX+NO2+CO+HO2]=CONST(J56*10)
k[MACRNCO3+HO2-->ACETOL+NO2+OH]=CONST(KAPHO2*0.44)
k[MACRNCO3+HO2-->MACRNCO2H+O3]=CONST(KAPHO2*0.15)
k[MACRNCO3+HO2-->MACRNCO3H]=CONST(KAPHO2*0.41)
k[MACRNCO3+NO-->ACETOL+NO2+NO2]=CONST(KAPNO)
k[MACRNCO3+NO2-->MACRNPAN]=CONST(KFPAN)
k[MACRNCO3+NO3-->ACETOL+NO2+NO2]=CONST(KRO2NO3*1.74)
k[MACRNCO3-->ACETOL+NO2]=CONST(1.00D-11*0.7*RO2)
k[MACRNCO3-->MACRNCO2H]=CONST(1.00D-11*0.3*RO2)
k[IBUTALOH+OH-->IPRHOCO3]=CONST(1.4D-11)
k[IBUTALOH+hv-->CH3COCH3+HO2+HO2+CO]=CONST(J17)
k[MACRNBCO3+HO2-->MACRNBCO2H+O3]=CONST(KAPHO2*0.15)
k[MACRNBCO3+HO2-->MACRNBCO3H]=CONST(KAPHO2*0.41)
k[MACRNBCO3+HO2-->NOA+HO2+OH]=CONST(KAPHO2*0.44)
k[MACRNBCO3+NO-->NOA+HO2+NO2]=CONST(KAPNO)
k[MACRNBCO3+NO2-->MACRNBPAN]=CONST(KFPAN)
k[MACRNBCO3+NO3-->NOA+HO2+NO2]=CONST(KRO2NO3*1.74)
k[MACRNBCO3-->MACRNBCO2H]=CONST(1.00D-11*0.3*RO2)
k[MACRNBCO3-->NOA+HO2]=CONST(1.00D-11*0.7*RO2)
k[CHOMOHCO3+HO2-->CHOMOHCO3H]=CONST(KAPHO2*0.56)
k[CHOMOHCO3+HO2-->MGLYOX+HO2+OH]=CONST(KAPHO2*0.44)
k[CHOMOHCO3+NO-->MGLYOX+NO2+HO2]=CONST(KAPNO)
k[CHOMOHCO3+NO2-->CHOMOHPAN]=CONST(KFPAN)
k[CHOMOHCO3+NO3-->MGLYOX+NO2+HO2]=CONST(KRO2NO3*1.74)
k[CHOMOHCO3-->MGLYOX+HO2]=CONST(1.00D-11*RO2)
k[PR1O2HNO3+OH-->CHOPRNO3+OH]=CONST(1.69D-12)
k[PR1O2HNO3+OH-->PRONO3AO2]=CONST(1.90D-12*EXP(190/(T)))
k[PR1O2HNO3+hv-->PRONO3AO+OH]=CONST(J41)
k[PRONO3AO-->CHOPRNO3+HO2]=CONST(KROPRIM*O2)
k[CHOPRNO3+NO3-->PRNO3CO3+HNO3]=CONST(KNO3AL*2.4)
k[CHOPRNO3+OH-->PRNO3CO3]=CONST(3.55D-12)
k[CHOPRNO3+hv-->PROPALO+NO2]=CONST(J56*10)
k[PROPOLNO3+OH-->ACETOL+NO2]=CONST(9.16D-13)
k[PR2O2HNO3+OH-->NOA+OH]=CONST(3.47D-12)
k[PR2O2HNO3+OH-->PRONO3BO2]=CONST(1.90D-12*EXP(190/(T)))
k[PR2O2HNO3+hv-->PRONO3BO+OH]=CONST(J41)
k[PRONO3BO-->NOA+HO2]=CONST(KROSEC*O2)
k[NOA+OH-->MGLYOX+NO2]=CONST(6.70D-13)
k[NOA+hv-->CH3COCH2O+NO2]=CONST(J56)
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k[PROLNO3+OH-->CH3CHOHCHO+NO2]=CONST(1.71D-12)
k[HCOCH2O2+HO2-->HCOCH2OOH]=CONST(KRO2HO2*0.387)
k[HCOCH2O2+NO-->NO2+HCOCH2O]=CONST(KRO2NO)
k[HCOCH2O2+NO3-->HCOCH2O+NO2]=CONST(KRO2NO3)
k[HCOCH2O2-->GLYOX]=CONST(2.00D-12*0.2*RO2)
k[HCOCH2O2-->HCOCH2O]=CONST(2.00D-12*0.6*RO2)
k[HCOCH2O2-->HOCH2CHO]=CONST(2.00D-12*0.2*RO2)
k[CL+CH4-->CH3O2]=CONST(6.6D-12*EXP(-1240/(T)))
k[OH+CH4-->CH3O2]=CONST(1.85D-12*EXP(-1690/(T)))
k[HYPROPO2H+OH-->ACETOL+OH]=CONST(2.44D-11)
k[HYPROPO2H+OH-->HYPROPO2]=CONST(1.90D-12*EXP(190/(T)))
k[HYPROPO2H+hv-->HYPROPO+OH]=CONST(J41)
k[HYPROPO-->CH3CHO+HCHO+HO2]=CONST(2.00D+14*EXP(-6410/(T)))
k[PROPGLY+OH-->ACETOL+HO2]=CONST(1.20D-11*0.613)
k[PROPGLY+OH-->CH3CHOHCHO+HO2]=CONST(1.20D-11*0.387)
k[IPROPOLO2H+OH-->CH3CHOHCHO+OH]=CONST(1.83D-11)
k[IPROPOLO2H+OH-->IPROPOLO2]=CONST(1.90D-12*EXP(190/(T)))
k[IPROPOLO2H+hv-->IPROPOLO+OH]=CONST(J41)
k[IPROPOLO-->CH3CHO+HCHO+HO2]=CONST(2.00D+14*EXP(-5505/(T)))
k[CH3CHOHCHO+NO3-->CH3CHOHCO3+HNO3]=CONST(KNO3AL*2.4)
k[CH3CHOHCHO+OH-->CH3CHOHCO3]=CONST(1.7D-11)
k[CH3CHOHCHO+hv-->CH3CHO+HO2+CO+HO2]=CONST(J17)
k[CH3COCO2H+hv-->CH3CO3+HO2]=CONST(J34)
k[OH+CH3COCO2H-->CH3CO3]=CONST(8.0D-13)
k[CO2H3CO3+HO2-->CO2H3CO3H]=CONST(KAPHO2*0.56)
k[CO2H3CO3+HO2-->MGLYOX+HO2+OH]=CONST(KAPHO2*0.44)
k[CO2H3CO3+NO-->MGLYOX+HO2+NO2]=CONST(KAPNO)
k[CO2H3CO3+NO2-->C4PAN6]=CONST(KFPAN)
k[CO2H3CO3+NO3-->MGLYOX+HO2+NO2]=CONST(KRO2NO3*1.74)
k[CO2H3CO3-->MGLYOX+HO2]=CONST(1.00D-11*RO2)
k[HOCH2CHO+NO3-->HOCH2CO3+HNO3]=CONST(KNO3AL)
k[HOCH2CHO+OH-->GLYOX+HO2]=CONST(1.00D-11*0.200)
k[HOCH2CHO+OH-->HOCH2CO3]=CONST(1.00D-11*0.800)
k[HOCH2CHO+hv-->HO2+HCHO+HO2+CO]=CONST(J15)
k[CO2N3CHO+OH-->CO2N3CO3]=CONST(7.20D-12)
k[CO2N3CHO+hv-->GLYOX+CH3CO3+NO2]=CONST(J56*10)
k[HOCH2CO3+HO2-->HO2+HCHO+OH]=CONST(KAPHO2*0.44)
k[HOCH2CO3+HO2-->HOCH2CO2H+O3]=CONST(KAPHO2*0.15)
k[HOCH2CO3+HO2-->HOCH2CO3H]=CONST(KAPHO2*0.41)
k[HOCH2CO3+NO-->NO2+HO2+HCHO]=CONST(KAPNO)
k[HOCH2CO3+NO2-->PHAN]=CONST(KFPAN)
k[HOCH2CO3+NO3-->NO2+HO2+HCHO]=CONST(KRO2NO3*1.74)
k[HOCH2CO3-->HCHO+HO2]=CONST(1.00D-11*0.7*RO2)
k[HOCH2CO3-->HOCH2CO2H]=CONST(1.00D-11*0.3*RO2)
k[CO23C3CHO+hv-->CH3CO3+CO+CO+HO2]=CONST(J34)
k[CO23C3CHO+hv-->CH3CO3+HCOCO]=CONST(J35)
k[NO3+CO23C3CHO-->CH3CO3+CO+CO+HNO3]=CONST(KNO3AL*4.0)
k[OH+CO23C3CHO-->CH3CO3+CO+CO]=CONST(1.23D-11)
k[ACO3+HO2-->ACO2H+O3]=CONST(KAPHO2*0.15)
k[ACO3+HO2-->ACO3H]=CONST(KAPHO2*0.41)
k[ACO3+HO2-->HO2+CO+HCHO+OH]=CONST(KAPHO2*0.44)
k[ACO3+NO-->HO2+CO+HCHO+NO2]=CONST(KAPNO)
k[ACO3+NO2-->ACRPAN]=CONST(KFPAN)
k[ACO3+NO3-->HO2+CO+HCHO+NO2]=CONST(KRO2NO3*1.74)
k[ACO3-->ACO2H]=CONST(1.00D-11*0.3*RO2)
k[ACO3-->HO2+CO+HCHO]=CONST(1.00D-11*0.7*RO2)
k[HMGLOOA-->HMGLOO]=CONST(KDEC*0.24)
k[HMGLOOA-->HOCH2CHO]=CONST(KDEC*0.20)
k[HMGLOOA-->HOCH2CO3+HO2]=CONST(KDEC*0.20)
k[HMGLOOA-->OH+CO+HOCH2CO3]=CONST(KDEC*0.36)
k[HOCH2COCHO+hv-->HOCH2CO3+CO+HO2]=CONST(J34)
k[NO3+HOCH2COCHO-->HOCH2CO3+CO+HNO3]=CONST(KNO3AL*2.4)
k[OH+HOCH2COCHO-->HOCH2CO3+CO]=CONST(1.44D-11)
k[MVKOHAO2+HO2-->MVKOHAOOH]=CONST(KRO2HO2*0.625)
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k[MVKOHAO2+NO-->MVKOHANO3]=CONST(KRO2NO*0.017)
k[MVKOHAO2+NO-->MVKOHAO+NO2]=CONST(KRO2NO*0.983)
k[MVKOHAO2+NO3-->MVKOHAO+NO2]=CONST(KRO2NO3)
k[MVKOHAO2-->H13CO2CHO]=CONST(2.00D-12*RO2*0.2)
k[MVKOHAO2-->MVKOHAO]=CONST(2.00D-12*RO2*0.6)
k[MVKOHAO2-->MVKOHAOH]=CONST(2.00D-12*RO2*0.2)
k[MVKOHBO2+HO2-->MVKOHBOOH]=CONST(KRO2HO2*0.625)
k[MVKOHBO2+NO-->MVKOHBO+NO2]=CONST(KRO2NO)
k[MVKOHBO2+NO3-->MVKOHBO+NO2]=CONST(KRO2NO3)
k[MVKOHBO2-->H14CO23C4]=CONST(8.80D-13*RO2*0.2)
k[MVKOHBO2-->MVKOHAOH]=CONST(8.80D-13*RO2*0.2)
k[MVKOHBO2-->MVKOHBO]=CONST(8.80D-13*RO2*0.6)
k[OH+IEPOXA-->IEACHO+HO2]=CONST(8.40D-12)
k[C526O2+HO2-->C526OOH]=CONST(KRO2HO2*0.706)
k[C526O2+NO-->C526NO3]=CONST(KRO2NO*0.065)
k[C526O2+NO-->C526O+NO2]=CONST(KRO2NO*0.935)
k[C526O2+NO3-->C526O+NO2]=CONST(KRO2NO3)
k[C526O2-->C526O]=CONST(9.20D-14*RO2)
k[C526O2-->HMVKBOOH+CO+OH]=CONST(K14ISOM1)
k[M3F+NO3-->C4MDIAL+NO2]=CONST(1.90D-11)
k[M3F+O3-->M3FOOA]=CONST(2.00D-17)
k[M3F+OH-->C4MDIAL+HO2]=CONST(9.00D-11)
k[NC2OOA-->NC2OO]=CONST(KDEC*0.11)
k[NC2OOA-->OH+NO2+GLYOX]=CONST(KDEC*0.89)
k[ACLOOA-->ACLOO]=CONST(KDEC*0.11)
k[ACLOOA-->OH+HO2+MGLYOX]=CONST(KDEC*0.89)
k[NO3CH2CHO+NO3-->NO3CH2CO3+HNO3]=CONST(KNO3AL)
k[NO3CH2CHO+OH-->NO3CH2CO3]=CONST(3.40D-12)
k[NO3CH2CHO+hv-->NO2+HCOCH2O]=CONST(J56*4.3)
k[C536OOH+OH-->DHPMEK+CO+OH]=CONST(6.60D-11)
k[C536OOH+hv-->C3MDIALOOH+HCHO+OH+OH]=CONST(J41)
k[C536OOH+hv-->DHPMEK+CO+OH+HO2]=CONST(J17)
k[C536OOH+hv-->MGLYOX+HCOCH2OOH+OH+OH]=CONST(J41*2)
k[C536O-->MGLYOX+HCOCH2OOH+OH]=CONST(KDEC)
k[DHPMEK+OH-->BIACETOOH+OH]=CONST(2.92D-11*0.56)
k[DHPMEK+OH-->C4CO2OOH+OH]=CONST(2.92D-11*0.44)
k[DHPMEK+hv-->CH3CO3+HCOCH2OOH+OH]=CONST(J41)
k[DHPMEK+hv-->CH3CO3+HCOCH2OOH+OH]=CONST(J22)
k[DHPMEK+hv-->MGLYOX+HCHO+OH+OH]=CONST(J41)
k[C5PACALD1+O3-->GLYOOC+CH3COCO3H]=CONST(2.40D-17*0.27)
k[C5PACALD1+O3-->GLYOX+PPACLOOA]=CONST(2.40D-17*0.73)
k[C5PACALD1+OH-->C534O2]=CONST(4.72D-11)
k[C5PACALD1+hv-->CH3CO3+GLYOX+OH]=CONST(J20*2)
k[MGLYOOA-->MGLYOO]=CONST(KDEC*0.11)
k[MGLYOOA-->OH+CO+CH3CO3]=CONST(KDEC*0.89)
k[HCOCH2OOH+OH-->GLYOX+OH]=CONST(2.91D-11)
k[HCOCH2OOH+OH-->HCOCH2O2]=CONST(1.90D-12*EXP(190/(T)))
k[HCOCH2OOH+hv-->HCOCH2O+OH]=CONST(J41)
k[HCOCH2OOH+hv-->HO2+CO+HCHO+OH]=CONST(J15)
k[PGAOOB-->GLYOX+OH+OH]=CONST(KDEC)
k[C4MALOHOOH+OH-->CO2H3CHO+CO+OH]=CONST(4.58D-11)
k[C4MALOHOOH+hv-->C4M2ALOHO+OH]=CONST(J41)
k[C4MALOHOOH+hv-->CO2H3CHO+HO2+CO+OH]=CONST(J17*2)
k[C4MDIAL+NO3-->C3MCODBCO3+HNO3]=CONST(KNO3AL*4.25)
k[C4MDIAL+NO3-->MC3CODBCO3+HNO3]=CONST(KNO3AL*4.25)
k[C4MDIAL+O3-->MGLYOOA+GLYOX]=CONST(5.00D-18*0.50)
k[C4MDIAL+O3-->MGLYOX+GLYOOC]=CONST(5.00D-18*0.50)
k[C4MDIAL+OH-->C3MCODBCO3]=CONST(4.41D-11*0.385)
k[C4MDIAL+OH-->C4M2ALOHO2]=CONST(4.41D-11*0.23)
k[C4MDIAL+OH-->MC3CODBCO3]=CONST(4.41D-11*0.385)
k[C4MDIAL+hv-->C3MCODBCO3+HO2+CO]=CONST(J4*0.2*0.3)
k[C4MDIAL+hv-->MC3CODBCO3+HO2+CO]=CONST(J4*0.2*0.3)
k[C4MDIAL+hv-->PXYFUONE]=CONST(J4*0.2*0.4)
k[HVMK+OH-->CO2H3CHO+HO2]=CONST(7.04D-11)
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k[HVMK+hv-->CO+HO2+MGLYOX+OH]=CONST(J20*0.5)
k[HC4ACO3+HO2-->ACETOL+CO+HO2+OH]=CONST(KAPHO2*0.44)
k[HC4ACO3+HO2-->HC4ACO2H+O3]=CONST(KAPHO2*0.15)
k[HC4ACO3+HO2-->HC4ACO3H]=CONST(KAPHO2*0.41)
k[HC4ACO3+NO-->ACETOL+CO+HO2+NO2]=CONST(KAPNO)
k[HC4ACO3+NO2-->C5PAN17]=CONST(KFPAN)
k[HC4ACO3+NO3-->ACETOL+CO+HO2+NO2]=CONST(KRO2NO3*1.74)
k[HC4ACO3-->ACETOL+HO2+CO]=CONST(1.00D-11*0.7*RO2)
k[HC4ACO3-->C5PACALD2+HO2]=CONST(2.20D10*EXP(-8174/(T))*EXP(1.00D8/(T)@3))
k[HC4ACO3-->HC4ACO2H]=CONST(1.00D-11*0.3*RO2)
k[GLYOOC-->GLYOO]=CONST(KDEC*0.11)
k[GLYOOC-->OH+HO2+CO+CO]=CONST(KDEC*0.89)
k[GLYOX+hv-->CO+CO+H2]=CONST(J31)
k[GLYOX+hv-->CO+CO+HO2+HO2]=CONST(J33)
k[GLYOX+hv-->HCHO+CO]=CONST(J32)
k[NO3+GLYOX-->HCOCO+HNO3]=CONST(KNO3AL)
k[OH+GLYOX-->HCOCO]=CONST(3.1D-12*EXP(340/(T)))
k[C58AO2+HO2-->C58AOOH]=CONST(KRO2HO2*0.706)
k[C58AO2+NO-->C58ANO3]=CONST(KRO2NO*0.065)
k[C58AO2+NO-->C58AO+NO2]=CONST(KRO2NO*0.935)
k[C58AO2+NO3-->C58AO+NO2]=CONST(KRO2NO3)
k[C58AO2-->C58AO]=CONST(8.80D-13*RO2)
k[C58AO2-->MACROH+CO+OH]=CONST(K14ISOM1)
k[OH+IEPOXB-->C57O2]=CONST(1.16D-11*0.370)
k[OH+IEPOXB-->C58AO2]=CONST(1.16D-11*0.370)
k[OH+IEPOXB-->C59O2]=CONST(1.16D-11*0.150)
k[OH+IEPOXB-->IEB1CHO]=CONST(1.16D-11*0.055)
k[OH+IEPOXB-->IEB4CHO]=CONST(1.16D-11*0.055)
k[MACRNOOA-->ACETOL+NO2+CO+OH]=CONST(KDEC*0.36)
k[MACRNOOA-->ACETOL+NO2+HO2]=CONST(KDEC*0.20)
k[MACRNOOA-->MACRNOO]=CONST(KDEC*0.24)
k[MACRNOOA-->PROPOLNO3]=CONST(KDEC*0.20)
k[INB1O2+HO2-->INB1OOH]=CONST(KRO2HO2*0.706)
k[INB1O2+NO-->INB1NO3]=CONST(KRO2NO*0.104)
k[INB1O2+NO-->INB1O+NO2]=CONST(KRO2NO*0.896)
k[INB1O2+NO3-->INB1O+NO2]=CONST(KRO2NO3)
k[INB1O2-->INB1CO]=CONST(2.90D-12*0.1*RO2)
k[INB1O2-->INB1O]=CONST(2.90D-12*0.8*RO2)
k[INB1O2-->INB1OH]=CONST(2.90D-12*0.1*RO2)
k[INB2O2+HO2-->INB2OOH]=CONST(KRO2HO2*0.706)
k[INB2O2+NO-->INANO3]=CONST(KRO2NO*0.087)
k[INB2O2+NO-->INB2O+NO2]=CONST(KRO2NO*0.913)
k[INB2O2-->C58NO3]=CONST(8.80D-13*0.2*RO2)
k[INB2O2-->INB1OH]=CONST(8.80D-13*0.2*RO2)
k[INB2O2-->INB2O]=CONST(8.80D-13*0.6*RO2)
k[OH+IEPOXC-->C59O2]=CONST(1.50D-11*0.719)
k[OH+IEPOXC-->IECCHO+HO2]=CONST(1.50D-11*0.281)
k[C527O2+HO2-->C527OOH]=CONST(KRO2HO2*0.706)
k[C527O2+NO-->C527NO3]=CONST(KRO2NO*0.065)
k[C527O2+NO-->C527O+NO2]=CONST(KRO2NO*0.935)
k[C527O2+NO3-->C527O+NO2]=CONST(KRO2NO3)
k[C527O2-->C527O]=CONST(8.80D-13*RO2)
k[C527O2-->MACROOH+CO+OH]=CONST(K14ISOM1)
k[GAOOB-->GAOO]=CONST(KDEC*0.11)
k[GAOOB-->OH+HO2+GLYOX]=CONST(KDEC*0.89)
k[NC3OOA-->NC3OO]=CONST(KDEC*0.11)
k[NC3OOA-->OH+NO2+MGLYOX]=CONST(KDEC*0.89)
k[INCO2+HO2-->INCOOH]=CONST(KRO2HO2*0.706)
k[INCO2+NO-->INCNO3]=CONST(KRO2NO*0.104)
k[INCO2+NO-->INCO+NO2]=CONST(KRO2NO*0.896)
k[INCO2+NO3-->INCO+NO2]=CONST(KRO2NO3)
k[INCO2-->INCCO]=CONST(2.90D-12*0.1*RO2)
k[INCO2-->INCO]=CONST(2.90D-12*0.8*RO2)
k[INCO2-->INCOH]=CONST(2.90D-12*0.1*RO2)
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k[C537OOH+OH-->DHPMPAL+CO+OH]=CONST(5.64D-11)
k[C537OOH+hv-->C4CO2OOH+HCHO+OH+OH]=CONST(J41)
k[C537OOH+hv-->DHPMPAL+CO+OH+HO2]=CONST(J17)
k[C537OOH+hv-->GLYOX+HYPERACET+OH+OH]=CONST(J41*2)
k[C537O-->GLYOX+HYPERACET+OH]=CONST(KDEC)
k[DHPMPAL+OH-->C3MDIALOOH+OH]=CONST(3.77D-11*0.32)
k[DHPMPAL+OH-->HYPERACET+CO+OH]=CONST(3.77D-11*0.68)
k[DHPMPAL+hv-->C3MDIALOOH+OH]=CONST(J41)
k[DHPMPAL+hv-->HYPERACET+OH+CO+HO2]=CONST(J15)
k[DHPMPAL+hv-->MGLYOX+OH+HCHO+OH]=CONST(J41)
k[C5PACALD2+O3-->MGLYOOA+HCOCO3H]=CONST(2.40D-17*0.73)
k[C5PACALD2+O3-->MGLYOX+PPGAOOB]=CONST(2.40D-17*0.27)
k[C5PACALD2+OH-->C535O2]=CONST(4.72D-11)
k[C5PACALD2+hv-->CO+HO2+MGLYOX+OH]=CONST(J20*2)
k[HYPERACET+OH-->CH3COCH2O2]=CONST(1.90D-12*EXP(190/(T)))
k[HYPERACET+OH-->MGLYOX+OH]=CONST(8.39D-12)
k[HYPERACET+hv-->CH3CO3+HCHO+OH]=CONST(J22)
k[HYPERACET+hv-->CH3COCH2O+OH]=CONST(J41)
k[PACLOOA-->MGLYOX+OH+OH]=CONST(KDEC)
k[HPC52O2+HO2-->HPC52OOH]=CONST(KRO2HO2*0.706)
k[HPC52O2+NO-->HPC52O+NO2]=CONST(KRO2NO)
k[HPC52O2+NO3-->HPC52O+NO2]=CONST(KRO2NO3)
k[HPC52O2-->HPC52O]=CONST(9.20D-14*RO2)
k[HMAC+OH-->C3MDIALOH+HO2]=CONST(5.56D-11)
k[HMAC+hv-->CO+HO2+MGLYOX+OH]=CONST(J20*0.5)
k[HC4CCO3+HO2-->CH3CO3+HOCH2CHO+OH]=CONST(KAPHO2*0.44)
k[HC4CCO3+HO2-->HC4CCO2H+O3]=CONST(KAPHO2*0.15)
k[HC4CCO3+HO2-->HC4CCO3H]=CONST(KAPHO2*0.41)
k[HC4CCO3+NO-->CH3CO3+HOCH2CHO+NO2]=CONST(KAPNO)
k[HC4CCO3+NO2-->C5PAN19]=CONST(KFPAN)
k[HC4CCO3+NO3-->CH3CO3+HOCH2CHO+NO2]=CONST(KRO2NO3*1.74)
k[HC4CCO3-->C5PACALD1+HO2]=CONST(8.14D9*EXP(-8591/(T))*EXP(1.00D8/(T)@3))
k[HC4CCO3-->CH3CO3+HOCH2CHO]=CONST(1.00D-11*0.7*RO2)
k[HC4CCO3-->HC4CCO2H]=CONST(1.00D-11*0.3*RO2)
k[C57AO2+HO2-->C57AOOH]=CONST(KRO2HO2*0.706)
k[C57AO2+NO-->C57AO+NO2]=CONST(KRO2NO*0.935)
k[C57AO2+NO-->INDHCHO]=CONST(KRO2NO*0.065)
k[C57AO2+NO3-->C57AO+NO2]=CONST(KRO2NO3)
k[C57AO2-->C57AO]=CONST(8.80D-13*RO2)
k[C57O2+HO2-->C57OOH]=CONST(KRO2HO2*0.706)
k[C57O2+NO-->C57NO3]=CONST(KRO2NO*0.019)
k[C57O2+NO-->C57O+NO2]=CONST(KRO2NO*0.981)
k[C57O2+NO3-->C57O+NO2]=CONST(KRO2NO3)
k[C57O2-->C57O]=CONST(9.20D-14*0.7*RO2)
k[C57O2-->C57OH]=CONST(9.20D-14*0.3*RO2)
k[C57O2-->HO12CO3C4+CO+OH]=CONST(K14ISOM1)
k[NC4OOA-->NC4OO]=CONST(KDEC*0.18)
k[NC4OOA-->OH+NO2+BIACETOH]=CONST(KDEC*0.82)
k[INDO2+HO2-->INDOOH]=CONST(KRO2HO2*0.706)
k[INDO2+NO-->INB1NO3]=CONST(KRO2NO*0.104)
k[INDO2+NO-->INDO+NO2]=CONST(KRO2NO*0.896)
k[INDO2+NO3-->INDO+NO2]=CONST(KRO2NO3)
k[INDO2-->INDO]=CONST(8.00D-13*0.8*RO2)
k[INDO2-->INDOH]=CONST(8.00D-13*0.2*RO2)
k[C59O2+HO2-->C59OOH]=CONST(KRO2HO2*0.706)
k[C59O2+NO-->C59O+NO2]=CONST(KRO2NO)
k[C59O2+NO3-->C59O+NO2]=CONST(KRO2NO3)
k[C59O2-->C59O]=CONST(9.20D-14*RO2)
k[INAOOH+hv-->INAO+OH]=CONST(J41)
k[OH+INAOOH-->INAHPCHO+HO2]=CONST(1.01D-11*0.65)
k[OH+INAOOH-->INAO2]=CONST(1.01D-11*0.35)
k[OH+INANO3-->ACETOL+NO2+NO3CH2CHO]=CONST(2.00D-12*0.07)
k[OH+INANO3-->C58NO3+NO2]=CONST(2.00D-12*0.39)
k[OH+INANO3-->HCHO+NO2+HMVKANO3]=CONST(2.00D-12*0.07)
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k[OH+INANO3-->INANCHO+HO2]=CONST(2.00D-12*0.33)
k[OH+INANO3-->INANCO+HO2]=CONST(2.00D-12*0.14)
k[INAO-->ACETOL+NO3CH2CHO+HO2]=CONST(KDEC)
k[OH+INAOH-->INAHCHO+HO2]=CONST(6.68D-12)
k[CO23C4NO3+OH-->CO23C3CHO+NO2]=CONST(1.30D-13)
k[CO23C4NO3+hv-->NO3CH2CO3+CH3CO3]=CONST(J35)
k[NC41OO+CO-->HMVKANO3]=CONST(1.20D-15)
k[NC41OO+NO-->HMVKANO3+NO2]=CONST(1.00D-14)
k[NC41OO+NO2-->HMVKANO3+NO3]=CONST(1.00D-15)
k[NC41OO+SO2-->HMVKANO3+SO3]=CONST(7.00D-14)
k[NC41OO-->HMVKANO3+H2O2]=CONST(6.00D-18*H2O)
k[C58OOH+hv-->C58O+OH]=CONST(J41)
k[OH+C58OOH-->C4MALOHOOH+HO2]=CONST(3.16D-11)
k[C58NO3+hv-->ACETOL+GLYOX+HO2+NO2]=CONST(J56*4)
k[OH+C58NO3-->C58NO3CO3]=CONST(2.32D-11)
k[C58O-->ACETOL+GLYOX+HO2]=CONST(KDEC)
k[OH+C58OH-->C58O]=CONST(3.04D-11)
k[HC4CO3H+OH-->HC4CO3]=CONST(9.11D-11)
k[HC4CO3H+hv-->MACR+HO2+OH]=CONST(J41)
k[HC4PAN+OH-->MACR+CO+NO2]=CONST(8.75D-11)
k[HC4PAN-->HC4CO3+NO2]=CONST(KBPAN)
k[CO2C3CO3H+OH-->CO2C3CO3]=CONST(4.18D-12)
k[CO2C3CO3H+hv-->CH3COCH2O2+OH]=CONST(J41)
k[CO2C3CO3H+hv-->CH3COCH2O2+OH]=CONST(J22)
k[CO2C3PAN+OH-->MGLYOX+CO+NO2]=CONST(5.93D-13)
k[CO2C3PAN-->CO2C3CO3+NO2]=CONST(KBPAN)
k[CH3COCH2O-->CH3CO3+HCHO]=CONST(KDEC)
k[C4CO2OOH+OH-->CO23C3CHO+OH]=CONST(7.83D-11)
k[C4CO2OOH+hv-->C4CO2O+OH]=CONST(J41)
k[C4CO2OOH+hv-->CH3CO3+GLYOX+OH]=CONST(J22)
k[C4CO2OOH+hv-->HO2+CO+MGLYOX+OH]=CONST(J17)
k[C4CO2O-->GLYOX+CH3CO3]=CONST(KDEC*0.5)
k[C4CO2O-->MGLYOX+HO2+CO]=CONST(KDEC*0.5)
k[CO2C3CO2H+OH-->CH3COCH2O2]=CONST(1.14D-12)
k[CO24C4CHO+hv-->CO2C3CO3+CO+HO2]=CONST(J34)
k[NO3+CO24C4CHO-->CO2C3CO3+CO+HNO3]=CONST(KNO3AL*5.5)
k[OH+CO24C4CHO-->CO2C3CO3+CO]=CONST(1.33D-11)
k[ACRO2+HO2-->HOCHOCOOH]=CONST(KRO2HO2*0.52)
k[ACRO2+NO-->CHOCOHCO+NO2]=CONST(KRO2NO)
k[ACRO2+NO3-->CHOCOHCO+NO2]=CONST(KRO2NO3)
k[ACRO2-->CHOCOHCO]=CONST(8.8D-13*RO2*0.6)
k[ACRO2-->HOCH2CHO+CO+OH]=CONST(K14ISOM1)
k[ACRO2-->HOCH2COCHO]=CONST(8.8D-13*RO2*0.2)
k[ACRO2-->OCCOHCOH]=CONST(8.8D-13*RO2*0.2)
k[OCCOHCO2+HO2-->C32OH13CO+O3]=CONST(0.4*0.52*KRO2HO2)
k[OCCOHCO2+HO2-->OCCOHCOOH]=CONST(0.6*0.52*KRO2HO2)
k[OCCOHCO2+NO-->C42AOH]=CONST(0.05*KRO2NO)
k[OCCOHCO2+NO-->OCCOHCO+NO2]=CONST(0.95*KRO2NO)
k[OCCOHCO2+NO3-->C42AOH+NO2]=CONST(KRO2NO3)
k[OCCOHCO2-->C32OH13CO]=CONST(2.0D-12*RO2*0.2)
k[OCCOHCO2-->OCCOHCO]=CONST(2.0D-12*RO2*0.6)
k[OCCOHCO2-->OCCOHCOH]=CONST(2.0D-12*RO2*0.2)
k[C2H4+NO3-->ETHENO3O2]=CONST(3.3D-12*EXP(-2880/(T)))
k[C2H4+O3-->HCHO+CH2OOA]=CONST(9.1D-15*EXP(-2580/(T)))
k[C2H4+OH-->HOCH2CH2O2]=CONST(KMT15)
k[GLYOOB-->GLYOO]=CONST(KDEC*0.24)
k[GLYOOB-->HCHO]=CONST(KDEC*0.20)
k[GLYOOB-->HO2+HO2+CO]=CONST(KDEC*0.20)
k[GLYOOB-->OH+CO+CO+HO2]=CONST(KDEC*0.36)
k[C524O2+HO2-->C524OOH]=CONST(KRO2HO2*0.706)
k[C524O2+NO-->C524NO3]=CONST(KRO2NO*0.104)
k[C524O2+NO-->C524O+NO2]=CONST(KRO2NO*0.896)
k[C524O2+NO3-->C524O+NO2]=CONST(KRO2NO3)
k[C524O2-->C524CO]=CONST(2.90D-12*RO2*0.1)
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k[C524O2-->C524O]=CONST(2.90D-12*RO2*0.8)
k[C524O2-->C524OH]=CONST(2.90D-12*RO2*0.1)
k[C524O2-->HMACR+HCHO+OH]=CONST(1.88D11*EXP(-9752/(T)))
k[CONM2CO3+HO2-->CONM2CO2H+O3]=CONST(KAPHO2*0.15)
k[CONM2CO3+HO2-->CONM2CO3H]=CONST(KAPHO2*0.41)
k[CONM2CO3+HO2-->MGLYOX+NO2+OH]=CONST(KAPHO2*0.44)
k[CONM2CO3+NO-->MGLYOX+NO2+NO2]=CONST(KAPNO)
k[CONM2CO3+NO2-->CONM2PAN]=CONST(KFPAN)
k[CONM2CO3+NO3-->MGLYOX+NO2+NO2]=CONST(KRO2NO3*1.74)
k[CONM2CO3-->CONM2CO2H]=CONST(1.00D-11*0.3*RO2)
k[CONM2CO3-->MGLYOX+NO2]=CONST(1.00D-11*0.7*RO2)
k[MACRNCO2H+OH-->ACETOL+NO2]=CONST(1.34D-12*0.44)
k[MACRNCO2H+OH-->CONM2CO2H+HO2]=CONST(1.34D-12*0.15)
k[MACRNCO3H+OH-->CONM2CO3H+HO2]=CONST(4.42D-12*0.15)
k[MACRNCO3H+OH-->MACRNCO3]=CONST(4.42D-12*0.85)
k[MACRNCO3H+hv-->ACETOL+NO2+OH]=CONST(J41)
k[MACRNPAN+OH-->CONM2PAN+HO2]=CONST(8.21D-13)
k[MACRNPAN-->MACRNCO3+NO2]=CONST(KBPAN)
k[IPRHOCO3+HO2-->CH3COCH3+HO2+OH]=CONST(KAPHO2*0.44)
k[IPRHOCO3+HO2-->IPRHOCO2H+O3]=CONST(KAPHO2*0.15)
k[IPRHOCO3+HO2-->IPRHOCO3H]=CONST(KAPHO2*0.41)
k[IPRHOCO3+NO-->CH3COCH3+HO2+NO2]=CONST(KAPNO)
k[IPRHOCO3+NO2-->C4PAN5]=CONST(KFPAN)
k[IPRHOCO3+NO3-->CH3COCH3+HO2+NO2]=CONST(KRO2NO3*1.74)
k[IPRHOCO3-->CH3COCH3+HO2]=CONST(1.00D-11*RO2*0.7)
k[IPRHOCO3-->IPRHOCO2H]=CONST(1.00D-11*RO2*0.3)
k[MACRNBCO2H+OH-->COHM2CO2H+NO2]=CONST(1.23D-12*0.32)
k[MACRNBCO2H+OH-->NOA+HO2]=CONST(1.23D-12*0.68)
k[MACRNBCO3H+OH-->COHM2CO3H+NO2]=CONST(4.31D-12*0.09)
k[MACRNBCO3H+OH-->MACRNBCO3]=CONST(4.31D-12*0.91)
k[MACRNBCO3H+hv-->NOA+HO2+OH]=CONST(J41)
k[MACRNBPAN+OH-->COHM2PAN+NO2]=CONST(7.10D-13)
k[MACRNBPAN-->MACRNBCO3+NO2]=CONST(KBPAN)
k[CHOMOHCO3H+OH-->CHOMOHCO3]=CONST(6.99D-11)
k[CHOMOHCO3H+hv-->MGLYOX+OH+HO2]=CONST(J41)
k[CHOMOHCO3H+hv-->MGLYOX+OH+HO2]=CONST(J17)
k[CHOMOHPAN+OH-->MGLYOX+CO+NO2]=CONST(6.64D-11)
k[CHOMOHPAN-->CHOMOHCO3+NO2]=CONST(KBPAN)
k[PRNO3CO3+HO2-->CH3CHO+NO2+OH]=CONST(KAPHO2*0.44)
k[PRNO3CO3+HO2-->PRNO3CO2H+O3]=CONST(KAPHO2*0.15)
k[PRNO3CO3+HO2-->PRNO3CO3H]=CONST(KAPHO2*0.41)
k[PRNO3CO3+NO-->CH3CHO+NO2+NO2]=CONST(KAPNO)
k[PRNO3CO3+NO2-->PRNO3PAN]=CONST(KFPAN)
k[PRNO3CO3+NO3-->CH3CHO+NO2+NO2]=CONST(KRO2NO3*1.74)
k[PRNO3CO3-->CH3CHO+NO2]=CONST(1.00D-11*0.7*RO2)
k[PRNO3CO3-->PRNO3CO2H]=CONST(1.00D-11*0.3*RO2)
k[PROPALO-->CH3CHO+HO2+CO]=CONST(KDEC)
k[HCOCH2O-->HCHO+CO+HO2]=CONST(KDEC)
k[CH3CHOHCO3+HO2-->CH3CHO+HO2+OH]=CONST(KAPHO2*0.44)
k[CH3CHOHCO3+HO2-->IPROPOLPER]=CONST(KAPHO2*0.56)
k[CH3CHOHCO3+NO-->CH3CHO+HO2+NO2]=CONST(KAPNO)
k[CH3CHOHCO3+NO2-->IPROPOLPAN]=CONST(KFPAN)
k[CH3CHOHCO3+NO3-->CH3CHO+HO2+NO2]=CONST(KRO2NO3*1.74)
k[CH3CHOHCO3-->CH3CHO+HO2]=CONST(1.00D-11*RO2)
k[CO2H3CO3H+hv-->CH3CO3+HO2+HCOCO3H]=CONST(J22)
k[CO2H3CO3H+hv-->MGLYOX+HO2+OH]=CONST(J41)
k[OH+CO2H3CO3H-->CO2H3CO3]=CONST(7.34D-12)
k[C4PAN6-->CO2H3CO3+NO2]=CONST(KBPAN)
k[OH+C4PAN6-->MGLYOX+CO+NO2]=CONST(3.74D-12)
k[CO2N3CO3+HO2-->CO2N3CO3H]=CONST(KAPHO2*0.56)
k[CO2N3CO3+HO2-->MGLYOX+NO2+OH]=CONST(KAPHO2*0.44)
k[CO2N3CO3+NO-->MGLYOX+NO2+NO2]=CONST(KAPNO)
k[CO2N3CO3+NO2-->CO2N3PAN]=CONST(KFPAN)
k[CO2N3CO3+NO3-->MGLYOX+NO2+NO2]=CONST(KRO2NO3*1.74)
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k[CO2N3CO3-->MGLYOX+NO2]=CONST(1.00D-11*RO2)
k[HOCH2CO2H+OH-->HCHO+HO2]=CONST(2.73D-12)
k[HOCH2CO3H+OH-->HOCH2CO3]=CONST(6.19D-12)
k[HOCH2CO3H+hv-->HCHO+HO2+OH]=CONST(J41)
k[PHAN+OH-->HCHO+CO+NO2]=CONST(1.12D-12)
k[PHAN-->HOCH2CO3+NO2]=CONST(KBPAN)
k[HCOCO-->CO+CO+HO2]=CONST(7.00D11*EXP(-3160/(T)))
k[HCOCO-->CO+CO+HO2]=CONST(5.00D-12*O2)
k[HCOCO-->CO+OH]=CONST(5.00D-12*O2*3.2*(1-EXP(-550/(T))))
k[HCOCO-->HCOCO3]=CONST(5.00D-12*O2*3.2*EXP(-550/(T)))
k[OH+ACO2H-->HO2+CO+HCHO]=CONST(8.66D-12)
k[ACO3H+hv-->HO2+CO+HCHO+OH]=CONST(J41)
k[OH+ACO3H-->ACO3]=CONST(3.60D-12)
k[OH+ACO3H-->HOCH2CHO+CO+OH]=CONST(6.58D-12)
k[ACRPAN-->ACO3+NO2]=CONST(KBPAN)
k[OH+ACRPAN-->HOCH2CHO+CO+NO3]=CONST(1.47D-11)
k[HMGLOO+CO-->HOCH2COCHO]=CONST(1.20D-15)
k[HMGLOO+NO-->HOCH2COCHO+NO2]=CONST(1.00D-14)
k[HMGLOO+NO2-->HOCH2COCHO+NO3]=CONST(1.00D-15)
k[HMGLOO+SO2-->HOCH2COCHO+SO3]=CONST(7.00D-14)
k[HMGLOO-->HOCH2COCHO+H2O2]=CONST(6.00D-18*H2O)
k[HMGLOO-->HOCH2COCO2H]=CONST(1.00D-17*H2O)
k[MVKOHAOOH+OH-->H13CO2CHO+OH]=CONST(5.98D-11)
k[MVKOHAOOH+hv-->MVKOHAO+OH]=CONST(J41)
k[MVKOHAOOH+hv-->MVKOHAO+OH]=CONST(J22)
k[MVKOHANO3+OH-->H13CO2CHO+NO2]=CONST(4.37D-12)
k[MVKOHAO-->HOCH2COCHO+HCHO+HO2]=CONST(KDEC)
k[H13CO2CHO+hv-->HOCH2CHO+CO+HO2+HO2]=CONST(J15)
k[NO3+H13CO2CHO-->H13CO2CO3+HNO3]=CONST(KNO3AL*4.0)
k[OH+H13CO2CHO-->H13CO2CO3]=CONST(2.66D-11)
k[MVKOHAOH+OH-->H13CO2CHO+HO2]=CONST(2.10D-11)
k[MVKOHAOH+hv-->HOCH2CO3+HOCH2CHO+HO2]=CONST(J22)
k[MVKOHBOOH+OH-->H14CO23C4+OH]=CONST(4.39D-12)
k[MVKOHBOOH+hv-->HOCH2CHO+HOCH2CO3+OH]=CONST(J22)
k[MVKOHBOOH+hv-->MVKOHBO+OH]=CONST(J41)
k[MVKOHBO-->HOCH2CHO+HOCH2CO3]=CONST(KDEC)
k[H14CO23C4+OH-->H1CO23CHO+HO2]=CONST(4.44D-12)
k[H14CO23C4+hv-->HOCH2CO3+HOCH2CO3]=CONST(J35)
k[IEACHO+hv-->HMVKBO2+CO+HO2]=CONST(J17)
k[NO3+IEACHO-->IEACO3+HNO3]=CONST(KNO3AL*7.5)
k[OH+IEACHO-->IEACO3]=CONST(2.20D-11)
k[C526OOH+OH-->HMVKBOOH+CO+OH]=CONST(5.70D-11*0.46)
k[C526OOH+OH-->IEC2OOH+OH]=CONST(5.70D-11*0.54)
k[C526OOH+hv-->HMVKBOOH+CO+OH+HO2]=CONST(J17)
k[C526OOH+hv-->MGLYOX+HOCH2CHO+OH+OH]=CONST(J41*2)
k[C526NO3+OH-->HMVKBOOH+CO+NO2]=CONST(1.56D-11)
k[C526NO3+hv-->C526O+NO2]=CONST(J56*10)
k[C526O-->MGLYOX+HOCH2CHO+OH]=CONST(KDEC)
k[M3FOOA-->C531O2+OH]=CONST(KDEC*0.6)
k[M3FOOA-->M3FOO]=CONST(KDEC*0.4)
k[NC2OO+CO-->NO3CH2CHO]=CONST(1.2D-15)
k[NC2OO+NO-->NO3CH2CHO+NO2]=CONST(1.0D-14)
k[NC2OO+NO2-->NO3CH2CHO+NO3]=CONST(1.0D-15)
k[NC2OO+SO2-->NO3CH2CHO+SO3]=CONST(7.0D-14)
k[NC2OO-->NO3CH2CHO+H2O2]=CONST(6.0D-18*H2O)
k[NC2OO-->NO3CH2CO2H]=CONST(1.0D-17*H2O)
k[ACLOO+CO-->ACETOL]=CONST(1.2D-15)
k[ACLOO+NO-->ACETOL+NO2]=CONST(1.0D-14)
k[ACLOO+NO2-->ACETOL+NO3]=CONST(1.0D-15)
k[ACLOO+SO2-->ACETOL+SO3]=CONST(7.0D-14)
k[ACLOO-->ACETOL+H2O2]=CONST(6.0D-18*H2O)
k[NO3CH2CO3+HO2-->HCHO+NO2+OH]=CONST(KAPHO2*0.44)
k[NO3CH2CO3+HO2-->NO3CH2CO2H+O3]=CONST(KAPHO2*0.15)
k[NO3CH2CO3+HO2-->NO3CH2CO3H]=CONST(KAPHO2*0.41)
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k[NO3CH2CO3+NO-->HCHO+NO2+NO2]=CONST(KAPNO)
k[NO3CH2CO3+NO2-->NO3CH2PAN]=CONST(KFPAN)
k[NO3CH2CO3+NO3-->HCHO+NO2+NO2]=CONST(KRO2NO3*1.74)
k[NO3CH2CO3-->HCHO+NO2]=CONST(1.00D-11*0.7*RO2)
k[NO3CH2CO3-->NO3CH2CO2H]=CONST(1.00D-11*0.3*RO2)
k[C3MDIALOOH+OH-->C3MDIALO2]=CONST(1.35D-10)
k[C3MDIALOOH+hv-->C3MDIALO+OH]=CONST(J41)
k[C3MDIALOOH+hv-->MGLYOX+OH+HO2+CO]=CONST(J17*2)
k[BIACETOOH+hv-->BIACETO+OH]=CONST(J41)
k[BIACETOOH+hv-->BIACETO+OH]=CONST(J35)
k[OH+BIACETOOH-->BIACETO2]=CONST(1.90D-12*EXP(190/(T)))
k[OH+BIACETOOH-->CO23C3CHO+OH]=CONST(5.99D-12)
k[CH3COCO3H+OH-->CH3COCO3]=CONST(3.69D-12)
k[CH3COCO3H+hv-->CH3CO3+OH]=CONST(J41)
k[CH3COCO3H+hv-->CH3CO3+OH]=CONST(J35)
k[PPACLOOA-->CH3COCO3+OH]=CONST(KDEC)
k[C534O2+HO2-->C534OOH]=CONST(KRO2HO2*0.706)
k[C534O2+NO-->C534O+NO2]=CONST(KRO2NO)
k[C534O2+NO3-->C534O+NO2]=CONST(KRO2NO3)
k[C534O2-->C534O]=CONST(9.20D-14*RO2)
k[C4M2ALOHO-->GLYOX+MGLYOX+HO2]=CONST(KDEC)
k[C3MCODBCO3+HO2-->C3MCODBCO2+OH]=CONST(KAPHO2*0.44)
k[C3MCODBCO3+HO2-->C5PACALD1]=CONST(KAPHO2*0.56)
k[C3MCODBCO3+NO-->C3MCODBCO2+NO2]=CONST(KAPNO)
k[C3MCODBCO3+NO2-->C3MCODBPAN]=CONST(KFPAN)
k[C3MCODBCO3+NO3-->NO2+C3MCODBCO2]=CONST(KRO2NO3*1.74)
k[C3MCODBCO3-->C3MCODBCO2]=CONST(1.00D-11*RO2)
k[MC3CODBCO3+HO2-->C5PACALD2]=CONST(KAPHO2*0.41)
k[MC3CODBCO3+HO2-->MC3CODBCO2+OH]=CONST(KAPHO2*0.44)
k[MC3CODBCO3+HO2-->MC3ODBCO2H+O3]=CONST(KAPHO2*0.15)
k[MC3CODBCO3+NO-->MC3CODBCO2+NO2]=CONST(KAPNO)
k[MC3CODBCO3+NO2-->MC3CODBPAN]=CONST(KFPAN)
k[MC3CODBCO3+NO3-->MC3CODBCO2+NO2]=CONST(KRO2NO3*1.74)
k[MC3CODBCO3-->MC3CODBCO2]=CONST(1.00D-11*0.70*RO2)
k[MC3CODBCO3-->MC3ODBCO2H]=CONST(1.00D-11*0.30*RO2)
k[C4M2ALOHO2+HO2-->C4MALOHOOH]=CONST(KRO2HO2*0.706)
k[C4M2ALOHO2+NO-->C4M2ALOHO+NO2]=CONST(KRO2NO)
k[C4M2ALOHO2+NO3-->C4M2ALOHO+NO2]=CONST(KRO2NO3)
k[C4M2ALOHO2-->C4M2AL2OH]=CONST(9.20D-14*RO2*0.30)
k[C4M2ALOHO2-->C4M2ALOHO]=CONST(9.20D-14*RO2*0.70)
k[PXYFUONE+NO3-->NPXYFUO2]=CONST(1.00D-12)
k[PXYFUONE+O3-->OH+CO+MCOCOMOXO2]=CONST(8.00D-19)
k[PXYFUONE+OH-->PXYFUO2]=CONST(2.42D-11)
k[OH+HC4ACO2H-->ACETOL+CO+HO2]=CONST(2.52D-11)
k[HC4ACO3H+hv-->ACETOL+CO+HO2+OH]=CONST(J41)
k[OH+HC4ACO3H-->MACROH+CO+OH]=CONST(3.84D-11)
k[C5PAN17-->HC4ACO3+NO2]=CONST(KBPAN)
k[OH+C5PAN17-->MACROH+CO+NO3]=CONST(7.79D-11)
k[GLYOO+CO-->GLYOX]=CONST(1.2D-15)
k[GLYOO+NO-->GLYOX+NO2]=CONST(1.0D-14)
k[GLYOO+NO2-->GLYOX+NO3]=CONST(1.0D-15)
k[GLYOO+SO2-->GLYOX+SO3]=CONST(7.0D-14)
k[GLYOO-->GLYOX+H2O2]=CONST(6.0D-18*H2O)
k[GLYOO-->HCOCO2H]=CONST(1.0D-17*H2O)
k[C58AOOH+OH-->MACROH+CO+OH]=CONST(3.70D-11)
k[C58AOOH+hv-->C58AO+OH]=CONST(J41)
k[C58ANO3+OH-->C47CHO+HO2]=CONST(8.14D-12)
k[C58ANO3+hv-->GLYOX+ACETOL+HO2+NO2]=CONST(J56*10)
k[C58AO-->ACETOL+GLYOX+HO2]=CONST(KDEC)
k[IEB1CHO+OH-->C4M2ALOHO2]=CONST(2.01D-11)
k[IEB4CHO+OH-->C4M2ALOHO2]=CONST(2.01D-11)
k[MACRNOO+CO-->MACRNO3]=CONST(1.2D-15)
k[MACRNOO+NO-->MACRNO3+NO2]=CONST(1.0D-14)
k[MACRNOO+NO2-->MACRNO3+NO3]=CONST(1.0D-15)
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k[MACRNOO+SO2-->MACRNO3+SO3]=CONST(7.0D-14)
k[MACRNOO-->MACRNCO2H]=CONST(1.0D-17*H2O)
k[MACRNOO-->MACRNO3+H2O2]=CONST(6.0D-18*H2O)
k[INB1OOH+OH-->INB1CO+OH]=CONST(1.27D-11*0.35)
k[INB1OOH+OH-->INB1HPCHO+HO2]=CONST(1.27D-11*0.34)
k[INB1OOH+OH-->INB1O2]=CONST(1.27D-11*0.31)
k[INB1OOH+hv-->INB1O+OH]=CONST(J41)
k[INB1NO3+OH-->INB1NACHO+HO2]=CONST(1.63D-12*0.50)
k[INB1NO3+OH-->INB1NBCHO+HO2]=CONST(1.63D-12*0.50)
k[INB1O-->HOCH2CHO+ACETOL+NO2]=CONST(KDEC)
k[INB1CO+OH-->INB1GLYOX+HO2]=CONST(3.27D-12)
k[INB1CO+hv-->ACETOL+NO2+HOCH2CO3]=CONST(J56*1.6)
k[INB1OH+OH-->C58NO3+HO2]=CONST(6.65D-12*0.71)
k[INB1OH+OH-->INB1CO+HO2]=CONST(6.65D-12*0.29)
k[INB2OOH+OH-->C58NO3+OH]=CONST(1.59D-11*0.73)
k[INB2OOH+OH-->INB2O2]=CONST(1.59D-11*0.27)
k[INB2OOH+hv-->INB2O+OH]=CONST(J41)
k[INB2O-->C57NO3+HO2]=CONST(KDEC)
k[IECCHO+hv-->MACRO2+HO2+CO]=CONST(J15)
k[NO3+IECCHO-->IECCO3+HNO3]=CONST(KNO3AL*7.5)
k[OH+IECCHO-->IECCO3]=CONST(2.76D-11)
k[C527OOH+OH-->MACROOH+CO+OH]=CONST(4.74D-11)
k[C527OOH+hv-->GLYOX+ACETOL+OH+OH]=CONST(J41*2)
k[C527OOH+hv-->MACROOH+CO+OH+HO2]=CONST(J17)
k[C527NO3+OH-->MACROOH+CO+NO2]=CONST(1.18D-11)
k[C527NO3+hv-->C527O+NO2]=CONST(J56*10)
k[C527O-->GLYOX+ACETOL+OH]=CONST(KDEC)
k[GAOO+CO-->HOCH2CHO]=CONST(1.2D-15)
k[GAOO+NO-->HOCH2CHO+NO2]=CONST(1.0D-14)
k[GAOO+NO2-->HOCH2CHO+NO3]=CONST(1.0D-15)
k[GAOO+SO2-->HOCH2CHO+SO3]=CONST(7.0D-14)
k[GAOO-->HOCH2CHO+H2O2]=CONST(6.0D-18*H2O)
k[GAOO-->HOCH2CO2H]=CONST(1.0D-17*H2O)
k[NC3OO+CO-->NOA]=CONST(1.2D-15)
k[NC3OO+NO-->NOA+NO2]=CONST(1.0D-14)
k[NC3OO+NO2-->NOA+NO3]=CONST(1.0D-15)
k[NC3OO+SO2-->NOA+SO3]=CONST(7.0D-14)
k[NC3OO-->NOA+H2O2]=CONST(6.0D-18*H2O)
k[INCOOH+hv-->INCO+OH]=CONST(J41)
k[OH+INCOOH-->INCCO+OH]=CONST(3.31D-11*0.89)
k[OH+INCOOH-->INCO2]=CONST(3.31D-11*0.11)
k[OH+INCNO3-->INCCO+NO2]=CONST(1.98D-12*0.445)
k[OH+INCNO3-->INCNCHO+HO2]=CONST(1.98D-12*0.414)
k[OH+INCNO3-->NOA+HOCH2CHO+NO2]=CONST(1.98D-12*0.141)
k[INCO-->NOA+HO2+HOCH2CHO]=CONST(KDEC)
k[INCCO+hv-->C59O+NO2]=CONST(J56*0.91)
k[OH+INCCO-->INCGLYOX+HO2]=CONST(3.30D-12)
k[OH+INCOH-->INCCO+HO2]=CONST(1.53D-11)
k[HCOCO3H+hv-->HO2+CO+OH]=CONST(J41)
k[HCOCO3H+hv-->HO2+CO+OH]=CONST(J15)
k[OH+HCOCO3H-->HCOCO3]=CONST(1.58D-11)
k[PPGAOOB-->HCOCO3+OH]=CONST(KDEC)
k[C535O2+HO2-->C535OOH]=CONST(KRO2HO2*0.706)
k[C535O2+NO-->C535O+NO2]=CONST(KRO2NO)
k[C535O2+NO3-->C535O+NO2]=CONST(KRO2NO3)
k[C535O2-->C535O]=CONST(9.20D-14*RO2)
k[HPC52OOH+OH-->HPC52CO3]=CONST(4.40D-11)
k[HPC52OOH+hv-->HO2+DHPMPAL+HO2+CO]=CONST(J15)
k[HPC52OOH+hv-->HPC52O+OH]=CONST(J41*2)
k[HPC52O-->GLYOX+HYPERACET+HO2]=CONST(KDEC)
k[OH+HC4CCO2H-->CH3CO3+HOCH2CHO]=CONST(2.52D-11)
k[HC4CCO3H+hv-->HOCH2CHO+CH3CO3+OH]=CONST(J41)
k[OH+HC4CCO3H-->HO12CO3C4+CO+OH]=CONST(3.84D-11)
k[C5PAN19-->HC4CCO3+NO2]=CONST(KBPAN)
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k[OH+C5PAN19-->HO12CO3C4+CO+NO3]=CONST(7.79D-11)
k[C57AOOH+OH-->HMVKBOOH+CO+HO2]=CONST(4.50D-11)
k[C57AOOH+hv-->C57AO+OH]=CONST(J41)
k[C57AO-->HOCH2CHO+MGLYOX+HO2]=CONST(KDEC)
k[INDHCHO+OH-->INDHCO3]=CONST(2.27D-11)
k[INDHCHO+hv-->MGLYOX+HOCH2CHO+HO2+NO2]=CONST(J56*4)
k[C57OOH+hv-->C57O+OH]=CONST(J41)
k[OH+C57OOH-->HO12CO3C4+CO+OH]=CONST(3.16D-11)
k[C57NO3+OH-->C4M2ALOHNO3+HO2]=CONST(9.37D-12*0.54)
k[C57NO3+OH-->C57NO3CO3]=CONST(9.37D-12*0.46)
k[C57NO3+hv-->MGLYOX+HOCH2CHO+HO2+NO2]=CONST(J56*10)
k[C57O-->MGLYOX+HOCH2CHO+HO2]=CONST(KDEC)
k[OH+C57OH-->C57O]=CONST(3.04D-11)
k[NC4OO+CO-->MVKNO3]=CONST(1.2D-15)
k[NC4OO+NO-->MVKNO3+NO2]=CONST(1.0D-14)
k[NC4OO+NO2-->MVKNO3+NO3]=CONST(1.0D-15)
k[NC4OO+SO2-->MVKNO3+SO3]=CONST(7.0D-14)
k[NC4OO-->MVKNO3+H2O2]=CONST(6.0D-18*H2O)
k[INDOOH+OH-->INDHPCHO+HO2]=CONST(9.20D-12*0.61)
k[INDOOH+OH-->INDO2]=CONST(9.20D-12*0.39)
k[INDOOH+hv-->INDO+OH]=CONST(J41)
k[INDO-->ACETOL+HOCH2CHO+NO2]=CONST(1.80D+13*((T)/298)@1.7*EXP(-4733/(T)))
k[INDO-->HCHO+HO2+MVKNO3]=CONST(1.80D+13*((T)/298)@1.7*EXP(-4079/(T)))
k[INDOH+OH-->INDHCHO+HO2]=CONST(5.60D-12)
k[C59OOH+hv-->C59O+OH]=CONST(J41)
k[C59OOH+hv-->HOCH2CO3+ACETOL+OH]=CONST(J22)
k[OH+C59OOH-->C59O2]=CONST(3.60D-12)
k[OH+C59OOH-->IEC2OOH+HO2]=CONST(1.57D-11)
k[C59O-->ACETOL+HOCH2CO3]=CONST(KDEC)
k[INAHPCHO+hv-->HMVKANO3+OH+CO+HO2]=CONST(J17)
k[INAHPCHO+hv-->HMVKANO3+OH+CO+HO2]=CONST(J41)
k[OH+INAHPCHO-->INAHPCO3]=CONST(2.67D-11)
k[INANCHO+hv-->HMVKANO3+NO2+CO+HO2]=CONST(J56*10)
k[OH+INANCHO-->INANCO3]=CONST(4.22D-12)
k[INANCO+hv-->ACETOL+NO2+NO3CH2CO3]=CONST(J56*1.6)
k[OH+INANCO-->INANCOCHO+HO2]=CONST(1.21D-12*0.56)
k[OH+INANCO-->INB1GLYOX+NO2]=CONST(1.21D-12*0.44)
k[INAHCHO+hv-->HMVKANO3+HO2+CO+HO2]=CONST(J17)
k[OH+INAHCHO-->INAHCO3]=CONST(2.29D-11)
k[C58NO3CO3+HO2-->C58NO3CO2H+O3]=CONST(KAPHO2*0.15)
k[C58NO3CO3+HO2-->C58NO3CO3H]=CONST(KAPHO2*0.41)
k[C58NO3CO3+HO2-->MACRNO3+HO2+OH]=CONST(KAPHO2*0.44)
k[C58NO3CO3+NO-->MACRNO3+HO2+NO2]=CONST(KAPNO)
k[C58NO3CO3+NO2-->C58NO3PAN]=CONST(KFPAN)
k[C58NO3CO3-->C58NO3CO2H]=CONST(1.00D-11*0.3*RO2)
k[C58NO3CO3-->MACRNO3+HO2]=CONST(1.00D-11*0.7*RO2)
k[HOCHOCOOH+OH-->HOCH2COCHO+OH]=CONST(4.77D-11)
k[HOCHOCOOH+hv-->CHOCOHCO+OH]=CONST(J41)
k[CHOCOHCO-->HOCH2CHO+HO2+CO]=CONST(KDEC)
k[OCCOHCOH+OH-->A2PANOO]=CONST(6.22D-11)
k[C32OH13CO+OH-->HCOCOHCO3]=CONST(1.36D-10)
k[C32OH13CO+hv-->GLYOX+HO2+HO2+CO]=CONST(J15*2)
k[OCCOHCOOH+OH-->OCCOHCO2]=CONST(9.258E-11)
k[OCCOHCOOH+hv-->OCCOHCO+OH]=CONST(J41)
k[C42AOH+hv-->HO2+CO+HO2+NO3CH2CHO]=CONST(J15)
k[OH+C42AOH-->NMGLYOX+HO2]=CONST(2.92D-11)
k[OCCOHCO-->HCHO+GLYOX+HO2]=CONST(KDEC)
k[ETHENO3O2+HO2-->ETHO2HNO3]=CONST(KRO2HO2*0.387)
k[ETHENO3O2+NO-->ETHENO3O+NO2]=CONST(KRO2NO)
k[ETHENO3O2+NO3-->ETHENO3O+NO2]=CONST(KRO2NO3)
k[ETHENO3O2-->ETHENO3O]=CONST(6.00D-13*0.6*RO2)
k[ETHENO3O2-->ETHOHNO3]=CONST(6.00D-13*0.2*RO2)
k[ETHENO3O2-->NO3CH2CHO]=CONST(6.00D-13*0.2*RO2)
k[CH2OOA-->CH2OO]=CONST(KDEC*0.37)
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k[CH2OOA-->CO]=CONST(KDEC*0.50)
k[CH2OOA-->HO2+CO+OH]=CONST(KDEC*0.13)
k[HOCH2CH2O2+HO2-->HYETHO2H]=CONST(1.53D-13*EXP(1300/(T)))
k[HOCH2CH2O2+NO-->ETHOHNO3]=CONST(KRO2NO*0.005)
k[HOCH2CH2O2+NO-->HOCH2CH2O+NO2]=CONST(KRO2NO*0.995)
k[HOCH2CH2O2+NO3-->HOCH2CH2O+NO2]=CONST(KRO2NO3)
k[HOCH2CH2O2-->ETHGLY]=CONST(2*(KCH3O2*7.8D-14*EXP(1000/(T)))@0.5*RO2*0.2)
k[HOCH2CH2O2-->HOCH2CH2O]=CONST(2*(KCH3O2*7.8D-14*EXP(1000/(T)))@0.5*RO2*0.6)
k[HOCH2CH2O2-->HOCH2CHO]=CONST(2*(KCH3O2*7.8D-14*EXP(1000/(T)))@0.5*RO2*0.2)
k[C524OOH+OH-->C524CO+OH]=CONST(1.18D-10*0.22)
k[C524OOH+OH-->C524O2]=CONST(1.18D-10*0.03)
k[C524OOH+OH-->HIEPOXB+OH]=CONST(1.18D-10*0.75)
k[C524OOH+hv-->C524O+OH]=CONST(J41)
k[C524NO3+OH-->NC524O2]=CONST(2.94D-11)
k[C524NO3+hv-->C524O+NO2]=CONST(J54)
k[C524O-->HMACR+HCHO+HO2]=CONST(KDEC)
k[C524CO+OH-->C525O2]=CONST(4.21D-11)
k[C524CO+hv-->HOCH2CO3+HOCH2CO3+HCHO]=CONST(J24)
k[C524OH+OH-->C524CO+HO2]=CONST(7.78D-11)
k[HMACR+NO3-->HMACO3+HNO3]=CONST(3.40D-15)
k[HMACR+O3-->CH2OOA+HOCH2COCHO]=CONST(7.80D-19*0.5)
k[HMACR+O3-->HCHO+HMGLYOOA]=CONST(7.80D-19*0.5)
k[HMACR+OH-->HMACO3]=CONST(4.83D-11*0.376)
k[HMACR+OH-->HMACRO2]=CONST(4.83D-11*0.624)
k[CONM2CO2H+OH-->MGLYOX+NO2]=CONST(3.70D-12)
k[CONM2CO2H+hv-->CO+HO2+NO2+CH3COCO2H]=CONST(J56*10)
k[CONM2CO3H+OH-->CONM2CO3]=CONST(6.78D-12)
k[CONM2CO3H+hv-->CO+HO2+NO2+CH3COCO3H]=CONST(J56*10)
k[CONM2PAN+OH-->CH3COPAN+CO+NO2]=CONST(3.18D-12)
k[CONM2PAN-->CONM2CO3+NO2]=CONST(KBPAN)
k[CONM2PAN+hv-->CONM2CO3+NO2]=CONST(J56*10)
k[IPRHOCO2H+OH-->CH3COCH3+HO2]=CONST(1.72D-12)
k[IPRHOCO3H+hv-->CH3COCH3+HO2+OH]=CONST(J41)
k[OH+IPRHOCO3H-->IPRHOCO3]=CONST(4.80D-12)
k[C4PAN5-->IPRHOCO3+NO2]=CONST(KBPAN)
k[OH+C4PAN5-->CH3COCH3+CO+NO2]=CONST(4.75D-13)
k[COHM2CO2H+OH-->GLYOX+HO2]=CONST(2.16D-11)
k[COHM2CO2H+hv-->HCOCO2H+CO+HO2]=CONST(J17)
k[COHM2CO3H+OH-->COHM2CO3]=CONST(2.47D-11)
k[COHM2CO3H+hv-->GLYOX+HO2+OH]=CONST(J41)
k[COHM2CO3H+hv-->HCOCO3H+CO+HO2]=CONST(J17)
k[COHM2PAN+OH-->GLYOX+NO3]=CONST(2.11D-11)
k[COHM2PAN-->COHM2CO3+NO2]=CONST(KBPAN)
k[COHM2PAN+hv-->COHM2CO3+NO2]=CONST(J17)
k[PRNO3CO2H+OH-->CH3CHO+NO2]=CONST(3.14D-13)
k[PRNO3CO3H+OH-->PRNO3CO3]=CONST(3.77D-12)
k[PRNO3CO3H+hv-->CH3CHO+NO2+OH]=CONST(J41)
k[PRNO3PAN+OH-->CH3CHO+CO+NO2+NO2]=CONST(1.43D-13)
k[PRNO3PAN-->PRNO3CO3+NO2]=CONST(KBPAN)
k[IPROPOLPER+OH-->CH3CHOHCO3]=CONST(9.34D-12)
k[IPROPOLPER+hv-->CH3CHO+HO2+OH]=CONST(J41)
k[IPROPOLPAN+OH-->CH3CHO+CO+NO2]=CONST(2.34D-12)
k[IPROPOLPAN-->CH3CHOHCO3+NO2]=CONST(KBPAN)
k[CO2N3CO3H+OH-->CO2N3CO3]=CONST(4.11D-12)
k[CO2N3CO3H+hv-->MGLYOX+NO2+OH]=CONST(J41)
k[CO2N3PAN+OH-->CO2N3CO3]=CONST(5.10D-13)
k[CO2N3PAN-->CO2N3CO3+NO2]=CONST(KBPAN)
k[CO2N3PAN+hv-->CO2N3CO3+NO2]=CONST(J56*10)
k[HCOCO3+HO2-->HCOCO2H+O3]=CONST(KAPHO2*0.15)
k[HCOCO3+HO2-->HCOCO3H]=CONST(KAPHO2*0.41)
k[HCOCO3+HO2-->HO2+CO+OH]=CONST(KAPHO2*0.44)
k[HCOCO3+NO-->HO2+CO+NO2]=CONST(KAPNO)
k[HCOCO3+NO2-->HO2+CO+NO3]=CONST(KFPAN)
k[HCOCO3+NO3-->HO2+CO+NO2]=CONST(KRO2NO3*1.74)
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k[HCOCO3-->CO+HO2]=CONST(1.00D-11*0.7*RO2)
k[HCOCO3-->HCOCO2H]=CONST(1.00D-11*0.3*RO2)
k[HOCH2COCO2H+OH-->HOCH2CO3]=CONST(2.89D-12)
k[HOCH2COCO2H+hv-->HOCH2CO3+HO2]=CONST(J34)
k[H13CO2CO3+HO2-->H13CO2CO3H]=CONST(KAPHO2*0.56)
k[H13CO2CO3+HO2-->HOCH2COCHO+HO2+OH]=CONST(KAPHO2*0.44)
k[H13CO2CO3+NO-->HOCH2COCHO+HO2+NO2]=CONST(KAPNO)
k[H13CO2CO3+NO2-->C4PAN10]=CONST(KFPAN)
k[H13CO2CO3+NO3-->HOCH2COCHO+HO2+NO2]=CONST(KRO2NO3*1.74)
k[H13CO2CO3-->HOCH2COCHO+HO2]=CONST(1.00D-11*RO2)
k[H1CO23CHO+OH-->CO+CO+HOCH2CO3]=CONST(1.44D-11)
k[H1CO23CHO+hv-->CO+CO+HOCH2CO3+HO2]=CONST(J34)
k[H1CO23CHO+hv-->CO+CO+HOCH2CO3+HO2]=CONST(J35)
k[IEACO3+HO2-->HMVKBO2+OH]=CONST(KAPHO2*0.44)
k[IEACO3+HO2-->IEACO3H]=CONST(KAPHO2*0.56)
k[IEACO3+NO-->HMVKBO2+NO2]=CONST(KAPNO)
k[IEACO3+NO2-->IEAPAN]=CONST(KFPAN)
k[IEACO3+NO3-->HMVKBO2+NO2]=CONST(KRO2NO3*1.74)
k[IEACO3-->HMVKBO2]=CONST(1.00D-11*RO2)
k[IEC2OOH+hv-->BIACETOH+OH+CO+HO2]=CONST(J17)
k[IEC2OOH+hv-->MGLYOX+OH+HOCH2CO3]=CONST(J22)
k[OH+IEC2OOH-->BIACETOH+OH+CO]=CONST(2.73D-11)
k[C531O2+HO2-->C531OOH]=CONST(KRO2HO2*0.706)
k[C531O2+NO-->C531O+NO2]=CONST(KRO2NO)
k[C531O2+NO3-->C531O+NO2]=CONST(KRO2NO3)
k[C531O2-->C531O]=CONST(2.00D-12*RO2)
k[M3FOO+CO-->C532CO]=CONST(1.20D-15)
k[M3FOO+NO-->C532CO+NO2]=CONST(1.00D-14)
k[M3FOO+NO2-->C532CO+NO3]=CONST(1.00D-15)
k[M3FOO+SO2-->C532CO+SO3]=CONST(7.00D-14)
k[M3FOO-->C532CO+H2O2]=CONST(6.00D-18*H2O)
k[NO3CH2CO2H+OH-->HCHO+NO2]=CONST(1.68D-13)
k[NO3CH2CO3H+OH-->NO3CH2CO3]=CONST(3.63D-12)
k[NO3CH2CO3H+hv-->HCHO+NO2+OH]=CONST(J41)
k[NO3CH2PAN+OH-->HCHO+CO+NO2+NO2]=CONST(1.12D-14)
k[NO3CH2PAN-->NO3CH2CO3+NO2]=CONST(KBPAN)
k[C3MDIALO2+HO2-->C3MDIALOOH]=CONST(KRO2HO2*0.625)
k[C3MDIALO2+NO-->C3MDIALO+NO2]=CONST(KRO2NO)
k[C3MDIALO2+NO3-->C3MDIALO+NO2]=CONST(KRO2NO3)
k[C3MDIALO2-->C3MDIALO]=CONST(9.20D-14*RO2*0.7)
k[C3MDIALO2-->C3MDIALOH]=CONST(9.20D-14*RO2*0.3)
k[C3MDIALO-->MGLYOX+CO+HO2]=CONST(KDEC)
k[BIACETO-->CH3CO3+HCHO+CO]=CONST(KDEC)
k[BIACETO2+HO2-->BIACETOOH]=CONST(KRO2HO2*0.625)
k[BIACETO2+NO-->BIACETO+NO2]=CONST(KRO2NO)
k[BIACETO2+NO3-->BIACETO+NO2]=CONST(KRO2NO3)
k[BIACETO2-->BIACETO]=CONST(2.00D-12*0.6*RO2)
k[BIACETO2-->BIACETOH]=CONST(2.00D-12*0.2*RO2)
k[BIACETO2-->CO23C3CHO]=CONST(2.00D-12*0.2*RO2)
k[CH3COCO3+HO2-->CH3CO3+OH]=CONST(KAPHO2*0.44)
k[CH3COCO3+HO2-->CH3COCO3H]=CONST(KAPHO2*0.56)
k[CH3COCO3+NO-->CH3CO3+NO2]=CONST(KAPNO)
k[CH3COCO3+NO2-->CH3COPAN]=CONST(KFPAN)
k[CH3COCO3+NO3-->CH3CO3+NO2]=CONST(KRO2NO3*1.74)
k[CH3COCO3-->CH3CO3]=CONST(1.00D-11*RO2)
k[C534OOH+OH-->C534O2]=CONST(3.42D-11)
k[C534OOH+hv-->C534O+OH]=CONST(J41)
k[C534OOH+hv-->C534O+OH]=CONST(J15)
k[C534OOH+hv-->CO2H3CHO+OH+OH]=CONST(J41)
k[C534O-->CH3COCO3H+GLYOX+HO2]=CONST(KDEC)
k[C3MCODBCO2-->MGLYOX+HO2+CO]=CONST(KDEC*0.35)
k[C3MCODBCO2-->MMALANHY+HO2]=CONST(KDEC*0.65)
k[C3MCODBPAN+OH-->MGLYOX+CO+CO+NO2]=CONST(4.37D-11)
k[C3MCODBPAN-->C3MCODBCO3+NO2]=CONST(KBPAN)
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k[MC3CODBCO2-->GLYOX+CH3O2+CO]=CONST(KDEC*0.35)
k[MC3CODBCO2-->MMALANHY+HO2]=CONST(KDEC*0.65)
k[MC3ODBCO2H+OH-->MC3CODBCO2]=CONST(4.38D-11)
k[MC3ODBCO2H+hv-->CH3COCO2H+HO2+CO+HO2+CO]=CONST(J18)
k[MC3ODBCO2H+hv-->CH3COCO2H+HO2+CO+HO2+CO]=CONST(J19)
k[MC3CODBPAN+OH-->GLYOX+HCHO+CO+NO2]=CONST(4.37D-11)
k[MC3CODBPAN-->MC3CODBCO3+NO2]=CONST(KBPAN)
k[C4M2AL2OH+OH-->C4M2ALOHO]=CONST(5.70D-11)
k[C4M2AL2OH+hv-->CO2H3CHO+HO2+CO+HO2]=CONST(J17*2)
k[NPXYFUO2+HO2-->NPXYFUOOH]=CONST(KRO2HO2*0.706)
k[NPXYFUO2+NO-->NPXYFUO+NO2]=CONST(KRO2NO)
k[NPXYFUO2+NO3-->NPXYFUO+NO2]=CONST(KRO2NO3)
k[NPXYFUO2-->NPXYFUO]=CONST(9.20D-14*RO2)
k[MCOCOMOXO2+HO2-->MCOCOMOOOH]=CONST(KRO2HO2*0.625)
k[MCOCOMOXO2+NO-->MCOCOMOXO+NO2]=CONST(KRO2NO)
k[MCOCOMOXO2+NO3-->MCOCOMOXO+NO2]=CONST(KRO2NO3)
k[MCOCOMOXO2-->MCOCOMOXO]=CONST(2.00D-12*RO2)
k[PXYFUO2+HO2-->PXYFUOOH]=CONST(KRO2HO2*0.706)
k[PXYFUO2+NO-->PXYFUO+NO2]=CONST(KRO2NO)
k[PXYFUO2+NO3-->PXYFUO+NO2]=CONST(KRO2NO3)
k[PXYFUO2-->PXYFUO]=CONST(9.20D-14*RO2*0.70)
k[PXYFUO2-->PXYFUOH]=CONST(9.20D-14*RO2*0.30)
k[HCOCO2H+hv-->HO2+HO2+CO]=CONST(J34)
k[OH+HCOCO2H-->CO+HO2]=CONST(1.23D-11)
k[C47CHO+OH-->C47CO3]=CONST(2.49D-11)
k[C47CHO+hv-->GLYOX+MGLYOX+HO2+NO2]=CONST(J56*10)
k[INB1HPCHO+hv-->ACETOL+GLYOX+OH+NO2]=CONST(J56*4)
k[OH+INB1HPCHO-->INB1HPCO3]=CONST(2.41D-11)
k[INB1NACHO+hv-->ACETOL+GLYOX+NO2+NO2]=CONST(J56*10)
k[OH+INB1NACHO-->INB1NACO3]=CONST(1.85D-11)
k[INB1NBCHO+hv-->MVKNO3+NO2+CO+HO2]=CONST(J56*10)
k[OH+INB1NBCHO-->INB1NBCO3]=CONST(1.85D-11)
k[INB1GLYOX+OH-->MACRNCO3+CO]=CONST(1.35D-11)
k[INB1GLYOX+hv-->MACRNCO3+CO+HO2]=CONST(J34)
k[IECCO3+HO2-->IECCO3H]=CONST(KAPHO2*0.56)
k[IECCO3+HO2-->MACRO2+OH]=CONST(KAPHO2*0.44)
k[IECCO3+NO-->MACRO2+NO2]=CONST(KAPNO)
k[IECCO3+NO2-->IECPAN]=CONST(KFPAN)
k[IECCO3+NO3-->MACRO2+NO2]=CONST(KRO2NO3*1.74)
k[IECCO3-->MACRO2]=CONST(1.00D-11*RO2)
k[INCNCHO+OH-->INCGLYOX+NO2]=CONST(4.52D-12*0.19)
k[INCNCHO+OH-->INCNCO3]=CONST(4.52D-12*0.81)
k[INCNCHO+hv-->GLYOX+NOA+HO2+NO2]=CONST(J56*10)
k[INCGLYOX+hv-->MACRNBCO3+CO+HO2]=CONST(J34)
k[OH+INCGLYOX-->MACRNBCO3+CO]=CONST(1.34D-11)
k[C535OOH+OH-->C535O2]=CONST(3.42D-11)
k[C535OOH+hv-->C3MDIALOOH+OH+HO2]=CONST(J41)
k[C535OOH+hv-->C535O+OH]=CONST(J41)
k[C535OOH+hv-->CO2H3CO3H+OH+HO2+CO]=CONST(J15)
k[C535O-->HCOCO3H+MGLYOX+HO2]=CONST(KDEC)
k[HPC52CO3+HO2-->HO2+DHPMPAL+OH]=CONST(KAPHO2*0.44)
k[HPC52CO3+HO2-->HPC52CO3H]=CONST(KAPHO2*0.56)
k[HPC52CO3+NO-->HO2+DHPMPAL+NO2]=CONST(KAPNO)
k[HPC52CO3+NO2-->HPC52PAN]=CONST(KFPAN)
k[HPC52CO3+NO3-->HO2+DHPMPAL+NO2]=CONST(KRO2NO3*1.6)
k[HPC52CO3-->HO2+DHPMPAL]=CONST(1.00D-11*RO2)
k[INDHCO3+HO2-->INDHCO3H]=CONST(KAPHO2*0.56)
k[INDHCO3+HO2-->MVKNO3+HO2+OH]=CONST(KAPHO2*0.44)
k[INDHCO3+NO-->MVKNO3+HO2+NO2]=CONST(KAPNO)
k[INDHCO3+NO2-->INDHPAN]=CONST(KFPAN)
k[INDHCO3+NO3-->MVKNO3+HO2+NO2]=CONST(KRO2NO3*1.74)
k[INDHCO3-->MVKNO3+HO2]=CONST(1.00D-11*RO2)
k[C4M2ALOHNO3+OH-->MMALNACO3]=CONST(2.53D-11*0.86)
k[C4M2ALOHNO3+OH-->MMALNBCO3]=CONST(2.53D-11*0.14)
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k[C4M2ALOHNO3+hv-->MGLYOX+GLYOX+HO2+NO2]=CONST(J56*10)
k[C57NO3CO3+HO2-->C57NO3CO2H+O3]=CONST(KAPHO2*0.15)
k[C57NO3CO3+HO2-->C57NO3CO3H]=CONST(KAPHO2*0.41)
k[C57NO3CO3+HO2-->HO12CO3C4+NO2+OH]=CONST(KAPHO2*0.44)
k[C57NO3CO3+NO-->HO12CO3C4+NO2+NO2]=CONST(KAPNO)
k[C57NO3CO3+NO2-->C57NO3PAN]=CONST(KFPAN)
k[C57NO3CO3+NO3-->HO12CO3C4+NO2+NO2]=CONST(KRO2NO3*1.74)
k[C57NO3CO3+NO3-->MACRNO3+HO2+NO2]=CONST(KRO2NO3*1.74)
k[C57NO3CO3-->C57NO3CO2H]=CONST(1.00D-11*0.3*RO2)
k[C57NO3CO3-->HO12CO3C4+NO2]=CONST(1.00D-11*0.7*RO2)
k[INDHPCHO+OH-->INDHPCO3]=CONST(2.58D-11)
k[INDHPCHO+hv-->MGLYOX+HOCH2CHO+OH+NO2]=CONST(J56*4)
k[INAHPCO3+HO2-->HMVKANO3+OH+OH]=CONST(KAPHO2*0.44)
k[INAHPCO3+HO2-->INAHPCO2H+O3]=CONST(KAPHO2*0.15)
k[INAHPCO3+HO2-->INAHPCO3H]=CONST(KAPHO2*0.41)
k[INAHPCO3+NO-->HMVKANO3+OH+NO2]=CONST(KAPNO)
k[INAHPCO3+NO2-->INAHPPAN]=CONST(KFPAN)
k[INAHPCO3+NO3-->HMVKANO3+OH+NO2]=CONST(KRO2NO3*1.74)
k[INAHPCO3-->HMVKANO3+OH]=CONST(1.00D-11*0.7*RO2)
k[INAHPCO3-->INAHPCO2H]=CONST(1.00D-11*0.3*RO2)
k[INANCO3+HO2-->HMVKANO3+NO2+OH]=CONST(KAPHO2*0.44)
k[INANCO3+HO2-->INANCO2H+O3]=CONST(KAPHO2*0.15)
k[INANCO3+HO2-->INANCO3H]=CONST(KAPHO2*0.41)
k[INANCO3+NO-->HMVKANO3+NO2+NO2]=CONST(KAPNO)
k[INANCO3+NO2-->INANPAN]=CONST(KFPAN)
k[INANCO3+NO3-->HMVKANO3+NO2+NO2]=CONST(KRO2NO3*1.74)
k[INANCO3-->HMVKANO3+NO2]=CONST(1.00D-11*0.7*RO2)
k[INANCO3-->INANCO2H]=CONST(1.00D-11*0.3*RO2)
k[OH+INANCOCHO-->INANCOCO3]=CONST(3.79D-12)
k[INAHCO3+HO2-->HMVKANO3+HO2+OH]=CONST(KAPHO2*0.44)
k[INAHCO3+HO2-->INAHCO2H+O3]=CONST(KAPHO2*0.15)
k[INAHCO3+HO2-->INAHCO3H]=CONST(KAPHO2*0.41)
k[INAHCO3+NO-->HMVKANO3+HO2+NO2]=CONST(KAPNO)
k[INAHCO3+NO2-->INAHPAN]=CONST(KFPAN)
k[INAHCO3+NO3-->HMVKANO3+HO2+NO2]=CONST(KRO2NO3*1.74)
k[INAHCO3-->HMVKANO3+HO2]=CONST(1.00D-11*0.7*RO2)
k[INAHCO3-->INAHCO2H]=CONST(1.00D-11*0.3*RO2)
k[OH+C58NO3CO2H-->MMALNACO2H+HO2]=CONST(2.49D-12)
k[C58NO3CO3H+hv-->MACRNO3+HO2+OH]=CONST(J41)
k[OH+C58NO3CO3H-->C58NO3CO3]=CONST(5.57D-12*0.68)
k[OH+C58NO3CO3H-->MMALNACO3H+HO2]=CONST(5.57D-12*0.32)
k[C58NO3PAN-->C58NO3CO3+NO2]=CONST(KBPAN)
k[OH+C58NO3PAN-->MMALNAPAN+HO2]=CONST(1.97D-12)
k[A2PANOO+HO2-->A2PANO+OH]=CONST(KAPHO2*0.44)
k[A2PANOO+HO2-->C2OHOCO2H+O3]=CONST(KAPHO2*0.15)
k[A2PANOO+HO2-->C2OHOCOOH]=CONST(KAPHO2*0.41)
k[A2PANOO+NO-->A2PANO+NO2]=CONST(KAPNO)
k[A2PANOO+NO2-->A2PAN]=CONST(KFPAN)
k[A2PANOO+NO3-->A2PANO+NO2]=CONST(KRO2NO3*1.74)
k[A2PANOO-->A2PANO]=CONST(1.00E-11*0.7*RO2)
k[A2PANOO-->C2OHOCO2H]=CONST(1.00E-11*0.3*RO2)
k[HCOCOHCO3+HO2-->GLYOX+HO2+OH]=CONST(KAPHO2*0.44)
k[HCOCOHCO3+HO2-->HCOCOHCO3H]=CONST(KAPHO2*0.56)
k[HCOCOHCO3+NO-->GLYOX+HO2+NO2]=CONST(KAPNO)
k[HCOCOHCO3+NO2-->HCOCOHPAN]=CONST(KFPAN)
k[HCOCOHCO3+NO3-->GLYOX+HO2+NO2]=CONST(KRO2NO3*1.74)
k[HCOCOHCO3-->GLYOX+HO2]=CONST(1.00D-11*RO2)
k[NMGLYOX+hv-->NO2+HCHO+CO+CO+HO2]=CONST(J53)
k[NMGLYOX+hv-->NO3CH2CO3+CO+HO2]=CONST(J34)
k[NO3+NMGLYOX-->NO3CH2CO3+CO+HNO3]=CONST(KNO3AL*2.4)
k[OH+NMGLYOX-->NO3CH2CO3+CO]=CONST(1.24D-11)
k[ETHO2HNO3+OH-->ETHENO3O2]=CONST(1.90D-12*EXP(190/(T)))
k[ETHO2HNO3+OH-->NO3CH2CHO+OH]=CONST(1.62D-12)
k[ETHO2HNO3+hv-->ETHENO3O+OH]=CONST(J41)
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k[ETHENO3O-->NO2+HCHO+HCHO]=CONST(7.00D+03)
k[ETHENO3O-->NO3CH2CHO+HO2]=CONST(KROPRIM*O2)
k[ETHOHNO3+OH-->HOCH2CHO+NO2]=CONST(8.40D-13)
k[HYETHO2H+OH-->HOCH2CH2O2]=CONST(1.90D-12*EXP(190/(T)))
k[HYETHO2H+OH-->HOCH2CHO+OH]=CONST(1.38D-11)
k[HYETHO2H+hv-->HOCH2CH2O+OH]=CONST(J41)
k[HOCH2CH2O-->HO2+HCHO+HCHO]=CONST(9.50D+13*EXP(-5988/(T)))
k[HOCH2CH2O-->HO2+HOCH2CHO]=CONST(KROPRIM*O2)
k[ETHGLY+OH-->HOCH2CHO+HO2]=CONST(1.45D-11)
k[HIEPOXB+OH-->HIEB1O2]=CONST(1.31D-11*0.667)
k[HIEPOXB+OH-->HIEB2O2]=CONST(1.31D-11*0.333)
k[NC524O2+HO2-->NC524OOH]=CONST(KRO2HO2*0.706)
k[NC524O2+NO-->NC524NO3]=CONST(KRO2NO*0.072)
k[NC524O2+NO-->NC524O+NO2]=CONST(KRO2NO*0.928)
k[NC524O2+NO3-->NC524O+NO2]=CONST(KRO2NO3)
k[NC524O2-->NC524O]=CONST(8.00D-13*RO2*0.8)
k[NC524O2-->NC524OH]=CONST(8.00D-13*RO2*0.2)
k[C525O2+HO2-->C525OOH]=CONST(KRO2HO2*0.706)
k[C525O2+NO-->C525O+NO2]=CONST(KRO2NO)
k[C525O2+NO3-->C525O+NO2]=CONST(KRO2NO3)
k[C525O2-->C525O]=CONST(9.20D-14*RO2)
k[HMACO3+HO2-->HMACO2H+O3]=CONST(KAPHO2*0.15)
k[HMACO3+HO2-->HMACO3H]=CONST(KAPHO2*0.41)
k[HMACO3+HO2-->HOCH2CO3+HCHO+OH]=CONST(KAPHO2*0.44)
k[HMACO3+NO-->HOCH2CO3+HCHO+NO2]=CONST(KAPNO)
k[HMACO3+NO2-->HMPAN]=CONST(KFPAN)
k[HMACO3+NO3-->HOCH2CO3+HCHO+NO2]=CONST(KRO2NO3*1.74)
k[HMACO3-->HMACO2H]=CONST(1.00D-11*RO2*0.3)
k[HMACO3-->HOCH2CO3+HCHO]=CONST(1.00D-11*RO2*0.7)
k[HMGLYOOA-->HMGLYOO]=CONST(KDEC*0.18)
k[HMGLYOOA-->HOCH2CO3+CO+HO2]=CONST(KDEC*0.82)
k[HMACRO2+HO2-->HMACROOH]=CONST(KRO2HO2*0.625)
k[HMACRO2+NO-->HMACRO+NO2]=CONST(KRO2NO)
k[HMACRO2+NO3-->HMACRO+NO2]=CONST(KRO2NO3)
k[HMACRO2-->H13CO2C3+CO+OH]=CONST(K14ISOM1)
k[HMACRO2-->HMACRO]=CONST(9.20D-14*RO2*0.7)
k[HMACRO2-->HMACROH]=CONST(9.20D-14*RO2*0.3)
k[CH3COPAN+OH-->HCHO+CO+CO+NO2]=CONST(1.02D-13)
k[CH3COPAN-->CH3COCO3+NO2]=CONST(KBPAN)
k[COHM2CO3+HO2-->COHM2CO2H+O3]=CONST(KAPHO2*0.15)
k[COHM2CO3+HO2-->COHM2CO3H]=CONST(KAPHO2*0.41)
k[COHM2CO3+HO2-->GLYOX+HO2+OH]=CONST(KAPHO2*0.44)
k[COHM2CO3+NO-->GLYOX+HO2+NO2]=CONST(KAPNO)
k[COHM2CO3+NO2-->COHM2PAN]=CONST(KFPAN)
k[COHM2CO3+NO3-->GLYOX+HO2+NO2]=CONST(KRO2NO3*1.74)
k[COHM2CO3-->COHM2CO2H]=CONST(1.00D-11*0.3*RO2)
k[COHM2CO3-->GLYOX+HO2]=CONST(1.00D-11*0.7*RO2)
k[H13CO2CO3H+hv-->HOCH2COCHO+HO2+OH]=CONST(J41)
k[OH+H13CO2CO3H-->H13CO2CO3]=CONST(9.43D-12)
k[C4PAN10-->H13CO2CO3+NO2]=CONST(KBPAN)
k[OH+C4PAN10-->HOCH2COCHO+CO+NO2]=CONST(5.83D-12)
k[IEACO3H+hv-->HMVKBO2+OH]=CONST(J41)
k[OH+IEACO3H-->IEACO3]=CONST(4.81D-12)
k[IEAPAN-->IEACO3+NO2]=CONST(KBPAN)
k[OH+IEAPAN-->HMVKBO2+CO+NO2]=CONST(1.21D-12)
k[C531OOH+OH-->C531CO+OH]=CONST(2.31D-11)
k[C531OOH+hv-->C531O+OH]=CONST(J41)
k[C531OOH+hv-->C531O+OH]=CONST(J22)
k[C531O-->C31CO3+HCHO]=CONST(KDEC)
k[C532CO+OH-->C533O2]=CONST(1.37D-11)
k[C532CO+hv-->C31CO3+CH3O2]=CONST(J22)
k[MMALANHY+OH-->MMALANHYO2]=CONST(1.50D-12)
k[NPXYFUOOH+OH-->NPXYFUO2]=CONST(5.16D-12)
k[NPXYFUOOH+hv-->NPXYFUO+OH]=CONST(J41)
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k[NPXYFUO-->C23O3CCHO+NO2]=CONST(KDEC)
k[MCOCOMOOOH+OH-->MCOCOMOXO2]=CONST(2.00D-11)
k[MCOCOMOOOH+hv-->CH3CO3+HCHO+OH]=CONST(J22)
k[MCOCOMOOOH+hv-->MCOCOMOXO+OH]=CONST(J41)
k[MCOCOMOXO-->HCHO+CH3CO3]=CONST(KDEC)
k[PXYFUOOH+OH-->PXYFUO2]=CONST(2.78D-11)
k[PXYFUOOH+hv-->PXYFUO+OH]=CONST(J41)
k[PXYFUO-->C23O3CCHO+HO2]=CONST(KDEC)
k[PXYFUOH+OH-->PXYFUO]=CONST(2.44D-11)
k[C47CO3+HO2-->C47CO3H]=CONST(KAPHO2*0.56)
k[C47CO3+HO2-->CO2N3CHO+HO2+OH]=CONST(KAPHO2*0.44)
k[C47CO3+NO-->CO2N3CHO+HO2+NO2]=CONST(KAPNO)
k[C47CO3+NO2-->C47PAN]=CONST(KFPAN)
k[C47CO3+NO3-->CO2N3CHO+HO2+NO2]=CONST(KRO2NO3*1.6)
k[C47CO3-->CO2N3CHO+HO2]=CONST(1.00D-11*RO2)
k[INB1HPCO3+HO2-->INB1HPCO2H+O3]=CONST(KAPHO2*0.15)
k[INB1HPCO3+HO2-->INB1HPCO3H]=CONST(KAPHO2*0.41)
k[INB1HPCO3+HO2-->MACRNO3+OH+OH]=CONST(KAPHO2*0.44)
k[INB1HPCO3+NO-->MACRNO3+OH+NO2]=CONST(KAPNO)
k[INB1HPCO3+NO2-->INB1HPPAN]=CONST(KFPAN)
k[INB1HPCO3+NO3-->MACRNO3+OH+NO2]=CONST(KRO2NO3*1.74)
k[INB1HPCO3-->INB1HPCO2H]=CONST(1.00D-11*0.3*RO2)
k[INB1HPCO3-->MACRNO3+OH]=CONST(1.00D-11*0.7*RO2)
k[INB1NACO3+HO2-->INB1NACO2H+O3]=CONST(KAPHO2*0.15)
k[INB1NACO3+HO2-->INB1NACO3H]=CONST(KAPHO2*0.41)
k[INB1NACO3+HO2-->MACRNO3+NO2+OH]=CONST(KAPHO2*0.44)
k[INB1NACO3+NO-->MACRNO3+NO2+NO2]=CONST(KAPNO)
k[INB1NACO3+NO2-->INB1NAPAN]=CONST(KFPAN)
k[INB1NACO3+NO3-->MACRNO3+NO2+NO2]=CONST(KRO2NO3*1.74)
k[INB1NACO3-->INB1NACO2H]=CONST(1.00D-11*0.3*RO2)
k[INB1NACO3-->MACRNO3+NO2]=CONST(1.00D-11*0.7*RO2)
k[INB1NBCO3+HO2-->INB1NBCO2H+O3]=CONST(KAPHO2*0.15)
k[INB1NBCO3+HO2-->INB1NBCO3H]=CONST(KAPHO2*0.41)
k[INB1NBCO3+HO2-->MVKNO3+NO2+OH]=CONST(KAPHO2*0.44)
k[INB1NBCO3+NO-->MVKNO3+NO2+NO2]=CONST(KAPNO)
k[INB1NBCO3+NO2-->INB1NBPAN]=CONST(KFPAN)
k[INB1NBCO3+NO3-->MVKNO3+NO2+NO2]=CONST(KRO2NO3*1.74)
k[INB1NBCO3-->INB1NBCO2H]=CONST(1.00D-11*0.3*RO2)
k[INB1NBCO3-->MVKNO3+NO2]=CONST(1.00D-11*0.7*RO2)
k[IECCO3H+hv-->MACRO2+OH]=CONST(J41)
k[OH+IECCO3H-->IECCO3]=CONST(1.04D-11)
k[IECPAN-->IECCO3+NO2]=CONST(KBPAN)
k[OH+IECPAN-->MACRO2+CO+NO2]=CONST(6.80D-12)
k[INCNCO3+HO2-->INCNCO2H+O3]=CONST(KAPHO2*0.15)
k[INCNCO3+HO2-->INCNCO3H]=CONST(KAPHO2*0.41)
k[INCNCO3+HO2-->MACRNB+NO2+OH]=CONST(KAPHO2*0.44)
k[INCNCO3+NO-->MACRNB+NO2+NO2]=CONST(KAPNO)
k[INCNCO3+NO2-->INCNPAN]=CONST(KFPAN)
k[INCNCO3+NO3-->MACRNB+NO2+NO2]=CONST(KRO2NO3*1.74)
k[INCNCO3-->INCNCO2H]=CONST(1.00D-11*0.3*RO2)
k[INCNCO3-->MACRNB+NO2]=CONST(1.00D-11*0.7*RO2)
k[HPC52CO3H+OH-->HPC52CO3]=CONST(2.69D-11)
k[HPC52CO3H+hv-->HO2+DHPMPAL+OH]=CONST(J41*3)
k[HPC52PAN+OH-->DHPMPAL+CO+NO2]=CONST(2.33D-11)
k[HPC52PAN-->HPC52CO3+NO2]=CONST(KBPAN)
k[INDHCO3H+OH-->INDHCO3]=CONST(5.66D-12)
k[INDHCO3H+hv-->MVKNO3+OH+HO2]=CONST(J41)
k[INDHPAN+OH-->MVKNO3+NO3]=CONST(1.96D-12)
k[INDHPAN-->INDHCO3+NO2]=CONST(KBPAN)
k[MMALNACO3+HO2-->CONM2CHO+HO2+OH]=CONST(KAPHO2*0.44)
k[MMALNACO3+HO2-->MMALNACO2H+O3]=CONST(KAPHO2*0.15)
k[MMALNACO3+HO2-->MMALNACO3H]=CONST(KAPHO2*0.41)
k[MMALNACO3+NO-->CONM2CHO+HO2+NO2]=CONST(KAPNO)
k[MMALNACO3+NO2-->MMALNAPAN]=CONST(KFPAN)
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k[MMALNACO3+NO3-->CONM2CHO+HO2+NO2]=CONST(KRO2NO3*1.74)
k[MMALNACO3-->CONM2CHO+HO2]=CONST(1.00D-11*0.7*RO2)
k[MMALNACO3-->MMALNACO2H]=CONST(1.00D-11*0.3*RO2)
k[MMALNBCO3+HO2-->CO2H3CHO+NO2+OH]=CONST(KAPHO2*0.44)
k[MMALNBCO3+HO2-->MMALNBCO2H+O3]=CONST(KAPHO2*0.15)
k[MMALNBCO3+HO2-->MMALNBCO3H]=CONST(KAPHO2*0.41)
k[MMALNBCO3+NO-->CO2H3CHO+NO2+NO2]=CONST(KAPNO)
k[MMALNBCO3+NO2-->MMALNBPAN]=CONST(KFPAN)
k[MMALNBCO3+NO3-->CO2H3CHO+NO2+NO2]=CONST(KRO2NO3*1.74)
k[MMALNBCO3-->CO2H3CHO+NO2]=CONST(1.00D-11*0.7*RO2)
k[MMALNBCO3-->MMALNBCO2H]=CONST(1.00D-11*0.3*RO2)
k[C57NO3CO2H+OH-->MMALNBCO2H+HO2]=CONST(6.52D-12)
k[C57NO3CO3H+OH-->C57NO3CO3]=CONST(6.52D-12*0.39)
k[C57NO3CO3H+OH-->MMALNBCO3H+HO2]=CONST(6.52D-12*0.61)
k[C57NO3CO3H+hv-->HO12CO3C4+NO2+OH]=CONST(J41)
k[C57NO3PAN+OH-->MMALNBPAN+HO2]=CONST(6.00D-12)
k[C57NO3PAN-->C57NO3CO3+NO2]=CONST(KBPAN)
k[INDHPCO3+HO2-->INDHPCO3H]=CONST(KAPHO2*0.56)
k[INDHPCO3+HO2-->MVKNO3+OH+OH]=CONST(KAPHO2*0.44)
k[INDHPCO3+NO-->MVKNO3+OH+NO2]=CONST(KAPNO)
k[INDHPCO3+NO2-->INDHPPAN]=CONST(KFPAN)
k[INDHPCO3+NO3-->MVKNO3+OH+NO2]=CONST(KRO2NO3*1.74)
k[INDHPCO3-->MVKNO3+OH]=CONST(1.00D-11*RO2)
k[INAHPCO2H+hv-->HMVKANO3+OH+HO2]=CONST(J41)
k[OH+INAHPCO2H-->HMVKANO3+OH]=CONST(6.50D-12)
k[INAHPCO3H+hv-->HMVKANO3+OH+OH]=CONST(J41*2)
k[OH+INAHPCO3H-->INAHPCO3]=CONST(9.58D-12)
k[INAHPPAN-->INAHPCO3+NO2]=CONST(KBPAN)
k[INAHPPAN+hv-->INAHPCO3+NO2]=CONST(J41)
k[OH+INAHPPAN-->HMVKANO3+OH+CO+NO2]=CONST(5.98D-12)
k[OH+INANCO2H-->HMVKANO3+NO2]=CONST(1.36D-12)
k[INANCO3H+hv-->HMVKANO3+NO2+OH]=CONST(J41)
k[OH+INANCO3H-->INANCO3]=CONST(4.08D-12)
k[INANPAN-->INANCO3+NO2]=CONST(KBPAN)
k[OH+INANPAN-->HMVKANO3+NO2+CO+NO2]=CONST(4.85D-13)
k[INANCOCO3+HO2-->INANCOCO2H+O3]=CONST(KAPHO2*0.15)
k[INANCOCO3+HO2-->INANCOCO3H]=CONST(KAPHO2*0.41)
k[INANCOCO3+HO2-->NO2+CO23C4NO3+OH]=CONST(KAPHO2*0.44)
k[INANCOCO3+NO-->NO2+CO23C4NO3+NO2]=CONST(KAPNO)
k[INANCOCO3+NO2-->INANCOPAN]=CONST(KFPAN)
k[INANCOCO3+NO3-->NO2+CO23C4NO3+NO2]=CONST(KRO2NO3*1.74)
k[INANCOCO3-->INANCOCO2H]=CONST(1.00D-11*0.3*RO2)
k[INANCOCO3-->NO2+CO23C4NO3]=CONST(1.00D-11*0.7*RO2)
k[OH+INAHCO2H-->HMVKANO3+HO2]=CONST(3.04D-12)
k[INAHCO3H+hv-->HMVKANO3+HO2+OH]=CONST(J41)
k[OH+INAHCO3H-->INAHCO3]=CONST(6.12D-12)
k[INAHPAN-->INAHPCO3+NO2]=CONST(KBPAN)
k[OH+INAHPAN-->HMVKANO3+HO2+CO+NO2]=CONST(2.52D-12)
k[MMALNACO2H+OH-->CONM2CHO+HO2]=CONST(4.93D-12)
k[MMALNACO2H+hv-->MGLYOX+NO2+HCOCO2H+HO2]=CONST(J56*10)
k[MMALNACO3H+OH-->MMALNACO3]=CONST(8.01D-12)
k[MMALNACO3H+hv-->MGLYOX+NO2+HCOCO3H+HO2]=CONST(J56*10)
k[MMALNAPAN+OH-->CONM2CHO+HO2+NO3]=CONST(4.41D-12)
k[MMALNAPAN-->MMALNACO3+NO2]=CONST(KBPAN)
k[MMALNAPAN+hv-->MMALNACO3+NO2]=CONST(J56*10)
k[A2PANO-->HOCH2CHO+HO2]=CONST(KDEC)
k[C2OHOCO2H+OH-->C3DIOLO2]=CONST(1.867E-11)
k[C2OHOCOOH+OH-->A2PANOO]=CONST(1.513E-11)
k[C2OHOCOOH+hv-->C3DIOLO2]=CONST(J41)
k[A2PAN+OH-->HOCH2CHO+CO+NO2]=CONST(1.865E-11)
k[A2PAN-->A2PANOO+NO2]=CONST(KBPAN)
k[HCOCOHCO3H+OH-->HCOCOHCO3]=CONST(7.33D-11)
k[HCOCOHCO3H+hv-->GLYOX+HO2+OH]=CONST(J41)
k[HCOCOHPAN+OH-->GLYOX+CO+NO2]=CONST(6.97D-11)
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k[HCOCOHPAN-->HCOCOHCO3+NO2]=CONST(KBPAN)
k[HIEB1O2+HO2-->HIEB1OOH]=CONST(KRO2HO2*0.706)
k[HIEB1O2+NO-->HIEB1O+NO2]=CONST(KRO2NO)
k[HIEB1O2+NO3-->HIEB1O+NO2]=CONST(KRO2NO3)
k[HIEB1O2-->HIEB1O]=CONST(9.20D-14*RO2)
k[HIEB2O2+HO2-->HIEB2OOH]=CONST(KRO2HO2*0.706)
k[HIEB2O2+NO-->HIEB2O+NO2]=CONST(KRO2NO)
k[HIEB2O2+NO3-->HIEB2O+NO2]=CONST(KRO2NO3)
k[HIEB2O2-->HIEB2O]=CONST(8.80D-13*RO2)
k[NC524OOH+OH-->HPNC524CO+HO2]=CONST(1.32D-11*0.728)
k[NC524OOH+OH-->NC524O2]=CONST(1.32D-11*0.272)
k[NC524OOH+hv-->NC524O+OH]=CONST(J41)
k[NC524NO3+OH-->DNC524CO+HO2]=CONST(2.43D-12)
k[NC524O-->HMVKNO3+HCHO+HO2]=CONST(1.80D+13*((T)/298)@1.7*EXP(-4079/(T)))
k[NC524O-->HOCH2CHO+NO2+H13CO2C3]=CONST(1.80D+13*((T)/298)@1.7*EXP(-4733/(T)))
k[NC524OH+OH-->HNC524CO+HO2]=CONST(9.60D-12)
k[C525OOH+OH-->C525O2]=CONST(1.37D-11)
k[C525OOH+hv-->C525O+OH]=CONST(J41)
k[C525O-->HOCH2CO3+H13CO2C3]=CONST(KDEC)
k[HMACO2H+OH-->HOCH2CO3+HCHO]=CONST(1.84D-11)
k[HMACO3H+OH-->H13CO2C3+CO+OH]=CONST(1.63D-11)
k[HMACO3H+OH-->HMACO3]=CONST(3.60D-12)
k[HMACO3H+hv-->HOCH2CO3+HCHO+OH]=CONST(J41)
k[HMPAN+OH-->H13CO2C3+CO+NO3]=CONST(2.90D-11)
k[HMPAN-->HMACO3+NO2]=CONST(KBPAN)
k[HMGLYOO+CO-->HOCH2COCHO]=CONST(1.20D-15)
k[HMGLYOO+NO-->HOCH2COCHO+NO2]=CONST(1.00D-14)
k[HMGLYOO+NO2-->HOCH2COCHO+NO3]=CONST(1.00D-15)
k[HMGLYOO+SO2-->HOCH2COCHO+SO3]=CONST(7.00D-14)
k[HMGLYOO-->HOCH2COCHO+H2O2]=CONST(6.00D-18*H2O)
k[HMACROOH+OH-->HMACRO2]=CONST(4.17D-11)
k[HMACROOH+hv-->H13CO2C3+CO+HO2+OH]=CONST(J17)
k[HMACROOH+hv-->HMACRO+OH]=CONST(J41)
k[HMACRO-->H13CO2C3+CO+HO2]=CONST(KDEC)
k[H13CO2C3+OH-->HOCH2COCHO+HO2]=CONST(5.25D-12)
k[H13CO2C3+hv-->HOCH2CO3+HCHO+HO2]=CONST(J22)
k[HMACROH+OH-->HMACRO]=CONST(3.82D-11)
k[HMACROH+hv-->H13CO2C3+CO+HO2+HO2]=CONST(J17)
k[C531CO+OH-->C31CO3+CO]=CONST(2.62D-11)
k[C531CO+hv-->C31CO3+CO+HO2]=CONST(J34)
k[C31CO3+HO2-->C31CO3H]=CONST(KAPHO2*0.56)
k[C31CO3+HO2-->CHOOCHO+CO+HO2+OH]=CONST(KAPHO2*0.44)
k[C31CO3+NO-->CHOOCHO+CO+HO2+NO2]=CONST(KAPNO)
k[C31CO3+NO2-->C31PAN]=CONST(KFPAN)
k[C31CO3+NO3-->CHOOCHO+CO+HO2+NO2]=CONST(KRO2NO3*1.6)
k[C31CO3-->CHOOCHO+CO+HO2]=CONST(1.00D-11*RO2)
k[C533O2+HO2-->C533OOH]=CONST(KRO2HO2*0.706)
k[C533O2+NO-->C533O+NO2]=CONST(KRO2NO)
k[C533O2+NO3-->C533O+NO2]=CONST(KRO2NO3)
k[C533O2-->C533O]=CONST(8.80D-13*RO2)
k[MMALANHYO2+HO2-->MMALNHYOOH]=CONST(KRO2HO2*0.706)
k[MMALANHYO2+NO-->MMALANHYO+NO2]=CONST(KRO2NO)
k[MMALANHYO2+NO3-->MMALANHYO+NO2]=CONST(KRO2NO3)
k[MMALANHYO2-->MMALANHYO]=CONST(9.20D-14*RO2*0.70)
k[MMALANHYO2-->MMALNHY2OH]=CONST(9.20D-14*RO2*0.30)
k[C23O3CCHO+NO3-->C23O3CCO3+HNO3]=CONST(KNO3AL*5.5)
k[C23O3CCHO+OH-->C23O3CCO3]=CONST(2.15D-11)
k[C23O3CCHO+hv-->CO+MCOCOMOXO2+HO2]=CONST(J15)
k[C47CO3H+OH-->C47CO3]=CONST(7.71D-12)
k[C47CO3H+hv-->GLYOX+CH3COCO3H+HO2+NO2]=CONST(J56*10)
k[C47PAN+OH-->CO2N3CHO+CO+NO3]=CONST(4.11D-12)
k[C47PAN-->C47CO3+NO2]=CONST(KBPAN)
k[C47PAN+hv-->C47CO3+NO2]=CONST(J56*10)
k[INB1HPCO2H+OH-->MACRNO3+OH]=CONST(7.40D-12)
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k[INB1HPCO3H+OH-->INB1HPCO3]=CONST(1.09D-11)
k[INB1HPCO3H+hv-->MACRNO3+OH+OH]=CONST(J41)
k[INB1HPPAN+OH-->MACRNO3+CO+OH+NO2]=CONST(7.26D-12)
k[INB1HPPAN-->INB1HPCO3+NO2]=CONST(KBPAN)
k[INB1NACO2H+OH-->MACRNO3+NO2]=CONST(1.72D-12)
k[INB1NACO3H+OH-->INB1NACO3]=CONST(5.18D-12)
k[INB1NACO3H+hv-->MACRNO3+NO2+OH]=CONST(J41)
k[INB1NAPAN+OH-->MACRNO3+CO+NO2+NO2]=CONST(1.58D-12)
k[INB1NAPAN-->INB1NACO3+NO2]=CONST(KBPAN)
k[INB1NBCO2H+OH-->MVKNO3+NO2]=CONST(1.73D-12)
k[INB1NBCO3H+OH-->INB1NBCO3]=CONST(5.19D-12)
k[INB1NBCO3H+hv-->MVKNO3+NO2+OH]=CONST(J41)
k[INB1NBPAN+OH-->MVKNO3+CO+NO2+NO2]=CONST(1.59D-12)
k[INB1NBPAN-->INB1NBCO3+NO2]=CONST(KBPAN)
k[OH+INCNCO2H-->MACRNB+NO2]=CONST(1.66D-12)
k[INCNCO3H+hv-->MACRNB+NO2+OH]=CONST(J41)
k[OH+INCNCO3H-->INCNCO3]=CONST(4.74D-12)
k[INCNPAN-->INCNCO3+NO2]=CONST(KBPAN)
k[OH+INCNPAN-->MACRNB+NO2+NO3]=CONST(1.14D-12)
k[MMALNBCO2H+OH-->CO2H3CHO+NO2]=CONST(2.23D-11)
k[MMALNBCO2H+hv-->GLYOX+CH3COCO2H+HO2+NO2]=CONST(J56*4)
k[MMALNBCO3H+OH-->MMALNBCO3]=CONST(2.59D-11)
k[MMALNBCO3H+hv-->GLYOX+CH3COCO3H+HO2+NO2]=CONST(J56*4)
k[MMALNBPAN+OH-->CO2H3CHO+NO2+NO3]=CONST(2.18D-11)
k[MMALNBPAN-->MMALNBCO3+NO2]=CONST(KBPAN)
k[MMALNBPAN+hv-->MMALNBCO3+NO2]=CONST(J56*4)
k[INDHPCO3H+OH-->INDHPCO3]=CONST(8.64D-12)
k[INDHPCO3H+hv-->MVKNO3+OH+OH]=CONST(J41*2)
k[INDHPPAN+OH-->MVKNO3+NO3]=CONST(5.04D-12)
k[INDHPPAN-->INDHPCO3+NO2]=CONST(KBPAN)
k[INDHPPAN+hv-->INDHPCO3+NO2]=CONST(J41)
k[INANCOCO2H+hv-->NO3CH2CO3+CH3COCO2H+NO2]=CONST(J56*1.6)
k[OH+INANCOCO2H-->NO2+CO23C4NO3]=CONST(9.35D-13)
k[INANCOCO3H+hv-->NO3CH2CO3+CH3COCO3H+NO2]=CONST(J56*1.6)
k[OH+INANCOCO3H-->INANCOCO3]=CONST(4.02D-12)
k[INANCOPAN+hv-->INANCOCO3+NO2]=CONST(J56*1.6)
k[INANCOPAN-->INANCOCO3+NO2]=CONST(KBPAN)
k[OH+INANCOPAN-->NO3+CO23C4NO3]=CONST(4.15D-13)
k[C3DIOLO2+HO2-->C3DIOLOOH]=CONST(KRO2HO2*0.520)
k[C3DIOLO2+NO-->C3DIOLO+NO2]=CONST(KRO2NO)
k[C3DIOLO2+NO3-->C3DIOLO+NO2]=CONST(KRO2NO3)
k[C3DIOLO2-->C3DIOLO]=CONST(2.00D-12*RO2)
k[HIEB1OOH+OH-->MVKOHAOH+CO+OH]=CONST(4.30D-11)
k[HIEB1OOH+hv-->HIEB1O+OH]=CONST(J41)
k[HIEB1OOH+hv-->MVKOHAOH+CO+OH+HO2]=CONST(J17)
k[HIEB1O-->HOCH2COCHO+HOCH2CHO+HO2]=CONST(KDEC)
k[HIEB2OOH+OH-->HMACROH+CO+OH]=CONST(5.74D-11)
k[HIEB2OOH+hv-->HIEB2O+OH]=CONST(J41)
k[HIEB2OOH+hv-->HMACROH+CO+OH+HO2]=CONST(J15)
k[HIEB2O-->H13CO2C3+GLYOX+HO2]=CONST(KDEC)
k[HPNC524CO+OH-->HMVKNO3+CO+OH]=CONST(2.98D-11)
k[HPNC524CO+hv-->HOCH2CHO+HOCH2COCHO+NO2+OH]=CONST(J56*4)
k[DNC524CO+OH-->HMVKNO3+CO+NO2]=CONST(1.93D-11)
k[DNC524CO+hv-->HMVKNO3+CO+HO2+NO2]=CONST(J56*4)
k[HMVKNO3+OH-->HMVKNGLYOX+HO2]=CONST(3.85D-12)
k[HMVKNO3+hv-->HOCH2CHO+NO2+CO+CO+HO2]=CONST(J56*1.6)
k[HNC524CO+OH-->HMVKNO3+CO+HO2]=CONST(2.67D-11)
k[HNC524CO+hv-->HOCH2CHO+HOCH2COCHO+NO2+HO2]=CONST(J56*4)
k[C31CO3H+OH-->C31CO3]=CONST(1.72D-11)
k[C31CO3H+hv-->CHOOCHO+CO+HO2+OH]=CONST(J41)
k[CHOOCHO+OH-->HO2+CO]=CONST(1.80D-13)
k[C31PAN+OH-->CHOOCHO+CO+NO3]=CONST(1.36D-11)
k[C31PAN-->C31CO3+NO2]=CONST(KBPAN)
k[C533OOH+OH-->C533O2]=CONST(2.20D-11)
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k[C533OOH+hv-->C533O+OH]=CONST(J41)
k[C533OOH+hv-->C533O+OH]=CONST(J22)
k[C533O-->CHOOCHO+MGLYOX+HO2]=CONST(KDEC)
k[MMALNHYOOH+OH-->MMALANHYO2]=CONST(1.69D-11)
k[MMALNHYOOH+hv-->MMALANHYO+OH]=CONST(J41)
k[MMALANHYO-->CO2H3CO3]=CONST(KDEC)
k[MMALNHY2OH+OH-->MMALANHYO]=CONST(1.34D-11)
k[C23O3CCO3+HO2-->C23O3CCO2H+O3]=CONST(KAPHO2*0.15)
k[C23O3CCO3+HO2-->C23O3CCO3H]=CONST(KAPHO2*0.41)
k[C23O3CCO3+HO2-->MCOCOMOXO2+OH]=CONST(KAPHO2*0.44)
k[C23O3CCO3+NO-->MCOCOMOXO2+NO2]=CONST(KAPNO)
k[C23O3CCO3+NO2-->C23O3CPAN]=CONST(KFPAN)
k[C23O3CCO3+NO3-->MCOCOMOXO2+NO2]=CONST(KRO2NO3*1.74)
k[C23O3CCO3-->C23O3CCO2H]=CONST(1.00D-11*RO2*0.3)
k[C23O3CCO3-->MCOCOMOXO2]=CONST(1.00D-11*RO2*0.7)
k[C3DIOLOOH+OH-->C3DIOLO2]=CONST(2.78D-11)
k[C3DIOLOOH+hv-->C3DIOLO+OH]=CONST(J41)
k[C3DIOLO-->HOCH2CHO+HCHO+HO2]=CONST(KDEC)
k[HMVKNGLYOX+OH-->CO+CO+HOCH2CHO+NO2]=CONST(1.36D-11)
k[HMVKNGLYOX+hv-->CO+CO+HOCH2CHO+NO2+HO2]=CONST(J34)
k[C23O3CCO2H+OH-->MCOCOMOXO2]=CONST(8.76D-13)
k[C23O3CCO3H+OH-->C23O3CCO3]=CONST(4.34D-12)
k[C23O3CCO3H+hv-->OH+MCOCOMOXO2]=CONST(J41)
k[C23O3CPAN+OH-->CO+C23O3CHO+NO2]=CONST(7.36D-13)
k[C23O3CPAN-->C23O3CCO3+NO2]=CONST(KBPAN)
k[C23O3CHO+NO3-->CO+CH3CO3+HNO3]=CONST(KNO3AL*4.0)
k[C23O3CHO+OH-->CO+CH3CO3]=CONST(1.27D-11)
k[C23O3CHO+hv-->CO+HO2+CH3CO3]=CONST(J22)
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