Supporting information for

Opinion: The Germicidal Effect of Ambient Air (Open Air Factor) Revisited

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1. Kinetics of ozone + alkene reactions inferred from data presented by Dark and Nash

Rate coefficients for the gas-phase reaction of ozone with alkenes used in the experiments by Dark and Nash (1970) can be estimated from the quantity of alkene needed to produce the ozone half-life of 5 minutes. The alkenes were in excess and dividing the pseudo first order loss rate of ozone (2.31×10^{-3} s^{-1}) by the alkene concentration used in the experiments gives the bimolecular rate coefficients shown on the y-axis in Fig. S1 below. Plotted on the x-axis are the rate coefficients taken from the 2020 recommendations by IUPAC (Cox et al., 2020) and McGillen et al. (2020). As seen from Fig. S1 the rate coefficients inferred from the experimental conditions reported by Dark and Nash in 1970 are consistent with our current understanding of the kinetics of ozone + alkene reactions, within about a factor of two. This consistency lends credibility to the experiments of Dark and Nash (1970) .

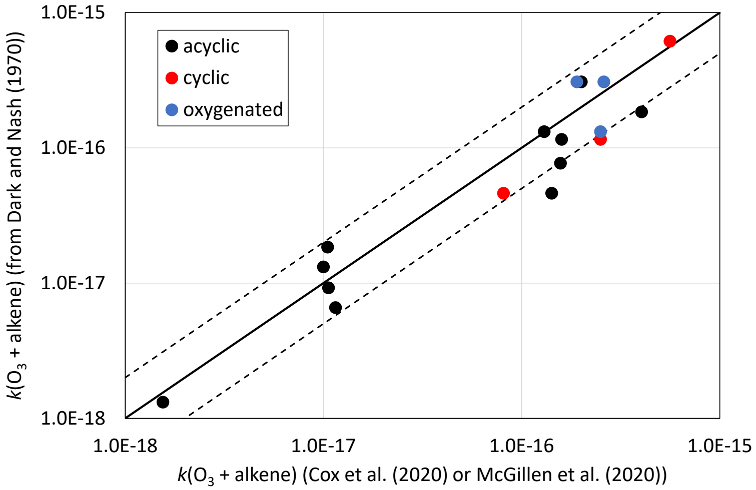


Figure S1. Rate coefficients for ozone + alkene reactions inferred from data presented by Dark and Nash (1970) plotted versus current recommendations for these reactions. The solid line represents 1:1 correspondence, the dotted lines show variation by a factor of two. The acyclic alkenes are ethene, propene, but-1-ene, pent-1-ene, hex-1-ene, *cis*-but-2-ene, *trans*-but-2-ene, *trans*-pent-2-ene*, *trans*-hex-2-ene*, 2-methylbut-2-ene, 2,4,4-trimethylpent-2-ene. The cyclic alkenes are cyclopentene, cyclohexene, and cycloheptene. The oxygenates are but-2-en-1-ol, 1-vinyloxyethane and 1-vinyloxybutane. (*Isomeric mixture used, which is dominated by *trans*- isomer).

2. Reanalysis of the data of Dark and Nash

The table below reproduces the experimental data of Dark and Nash (1970) for the selected alkenes presented in Fig. 1 of the main paper. The effects on the *Escherichia coli* population were reported as a survival fraction (*f*) following a 10 minute experimental exposure time, and a first-order loss rate constant, k_{loss} (in units of min^{-1}) is inferred here, representing the average removal rate over the 10 minute period.

Table S1. Survival fractions (*f*) of *Escherichia coli* reported by Dark and Nash (1970) for selected ozone-alkene experiments and the inferred loss rates (k_{loss}) of *Escherichia coli*.

	Survival fraction (*f*) [a]			**k_{loss}/min^{-1} [b]**		
$[O_3]_0$/ppb	33 ppb	11 ppb	4 ppb	33 ppb	11 ppb	4 ppb
cyclohexene	0.02	0.07	0.35	0.391	0.266	0.105
hex-2-ene [c]	0.05	0.20	0.70	0.300	0.161	0.036
pent-1-ene	0.05	0.20	0.65	0.300	0.161	0.043
pent-2-ene [c]	0.10	0.50	0.80	0.230	0.069	0.022
trans-but-2-ene	0.10	0.30	0.85	0.230	0.120	0.016
propene	0.20	0.70	0.70	0.161	0.036	0.036
hex-1-ene	0.20	0.70	0.75	0.161	0.036	0.029
cis-but-2-ene	0.20	0.75	1.00	0.161	0.029	0.000
but-1-ene	0.35	0.35	0.90	0.105	0.105	0.011
2-methylbut-2-ene	0.55	0.75	1.00	0.060	0.029	0.000
2,4,4-trimethylpent-2-ene	1.00	1.00	1.00	0.000	0.000	0.000

Notes:

[a] Survival fraction of *Escherichia coli* at the end of each 10 minute experiment, as reported by Dark and Nash (1970);

[b] The inferred average first-order loss rate, k_{loss}, determined from $k_{\mathrm{loss}} = \ln(1/f)/10$ and thus assumes that mixing of gases was rapid compared to the 10 minute timescale over which the *E-coli* were exposed.

[c] Isomeric mixture dominated by *trans* isomer.

3. Concentrations and Lifetime of sCI in outside air

Cox et al. (2020) have recently estimated seasonally-averaged winter and summer production rates, removal rates and steady-state concentrations of sCIs, using observational data from the Chilbolton Observatory (Hampshire, southern England), which is about 15 km to the east of MRE Porton Down and in a similarly rural location. Full details are available in section 8 and Supplement C of Cox et al. (2020). The calculations made use of measured or inferred concentrations of a series of C_1–C_6 alkenes, isoprene, α-pinene, limonene, O_3, NO_2, SO_2 and HC(O)OH, in conjunction with H_2O and $(H_2O)_2$ concentrations based on modelled temperature and relative humidity data typical of the region. Production of sCIs from the ozonolysis of the C_1–C_6 alkenes, isoprene, α-pinene and limonene was therefore represented, with removal by unimolecular decomposition and bimolecular reactions with H_2O, $(H_2O)_2$, NO_2, SO_2 and HC(O)OH. These are expected to be the most important source and sink reactions (Cox et al., 2020).

Table S2. Representative ambient concentrations and lifetimes of a core set of sCIs calculated by Cox et al. (2020) for average winter conditions at the Chilbolton observatory in south-east England (T = 278 K; RH = 85 %).

sCI	**Ambient concentration/ molecule cm^{-3}**	**Lifetime/ s**	**Main removal reaction**
CH_2OO	5.3	5.3×10^{-4}	Reaction with $(H_2O)_2$
Z-CH_3CHOO	300	1.5×10^{-2}	Thermal decomposition
E-CH_3CHOO	2.0	9.6×10^{-5}	Reaction with $(H_2O)_2$ and H_2O
$(CH_3)_2COO$	28	5.1×10^{-3}	Thermal decomposition
Z-$(CH{=}CH_2)(CH_3)COO$ [a]	0.010	2.8×10^{-4}	Thermal decomposition
E-$(CH{=}CH_2)(CH_3)COO$ [a]	4.9	5.8×10^{-2}	Thermal decomposition
Z-$(C(CH_3){=}CH_2)CHOO$ [a]	0.0042	2.7×10^{-4}	Thermal decomposition
E-$(C(CH_3){=}CH_2)CHOO$ [a]	0.57	1.6×10^{-2}	Reaction with $(H_2O)_2$ and H_2O

Notes:
[a] Derived specifically from isoprene.

Table S3. Representative ambient concentrations and lifetimes of a core set of sCIs calculated by Cox et al. (2020) for average summer conditions at the Chilbolton observatory in south-east England (T = 288 K; RH = 70 %).

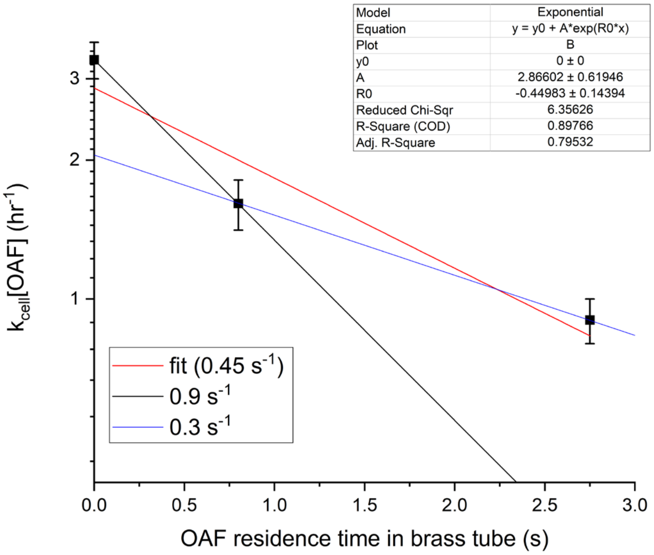
sCI	**Ambient concentration (molecule cm^{-3})**	**Lifetime (s)**	**Main removal reaction**
CH_2OO	4.5	4.2×10^{-4}	Reaction with $(H_2O)_2$
Z-CH_3CHOO	220	9.1×10^{-3}	Thermal decomposition
E-CH_3CHOO	1.5	6.0×10^{-5}	Reaction with $(H_2O)_2$ and H_2O
$(CH_3)_2COO$	19	3.4×10^{-3}	Thermal decomposition
Z-$(CH{=}CH_2)(CH_3)COO$ [a]	0.025	1.4×10^{-4}	Thermal decomposition
E-$(CH{=}CH_2)(CH_3)COO$ [a]	11	2.7×10^{-2}	Thermal decomposition
Z-$(C(CH_3){=}CH_2)CHOO$ [a]	0.010	1.3×10^{-4}	Thermal decomposition
E-$(C(CH_3){=}CH_2)CHOO$ [a]	1.3	7.7×10^{-3}	Reaction with $(H_2O)_2$ and H_2O

Notes:
[a] Derived specifically from isoprene.

Tables S2 and S3 show the calculated ambient concentrations and lifetimes of a core set of sCIs for winter and summer conditions, with the total sCI concentrations being about 380 molecule cm^{-3} in both summer and winter. The core set accounted for 91 % and 76 % of the winter and summer totals, with a particularly important contribution from *Z*-CH_3CHOO, which is formed from all linear alk-2-enes in the alkene speciation and has a relatively long atmospheric lifetime. The main sCI removal reactions were either thermal decomposition or reaction with $(H_2O)_2$ (supplemented by reaction with H_2O). The calculated ambient lifetimes for all sCIs were < 60 ms in the winter and < 30 ms in the summer, with many being orders of magnitude shorter lived.

4. Analysis of Druett and May's "Brass tube" experiment

Based on the information given by Druett and May (1968), the gas flow through the l = 12.8 m long and d = 11.4 cm inner diameter long brass tube was 171 m^3 h^{-1} giving a gas residence time 2.75 s. The spider webs with the bacterial cells were mounted at residence times of 0, 0.8 s and 2.75 s. The slope of the exponential decay of the viable cells as a function of the operation time of the flow tube at these positions was k_{cell} = 3.3 ± 0.3, 1.6 ± 0.2, and 0.9 ± 0.7 h^{-1}, respectively. Assuming that k_{cell} is linearly related to the OAF concentration, we can estimate the first order loss rate of OAF along the brass tube from a plot of k_{cell} as a function of the residence time in the brass tube, shown in Fig. S2. From Fig. S2 we see that the decay of bactericidal activity decreased non-exponentially, reasons for which could be manifold. First, the outdoor concentration of OAF (and its precursors) may have varied over time of operation of the flow tube. Second, the OAF is likely to be a group of individual species with variable life-times. Third, OAF may have been generated along the tube as the precursor chemistry continued. Rough values for the loss rate coefficients k_{OAF} from the first two points, the second and third points and all three combined are 0.9, 0.3 and 0.5 s^{-1}, respectively.



Model	Exponential
Equation	y = y0 + A*exp(R0*x)
Plot	B
y0	0 ± 0
A	2.86602 ± 0.61946
R0	-0.44983 ± 0.14394
Reduced Chi-Sqr	6.35626
R-Square (COD)	0.89766
Adj. R-Square	0.79532

Figure S2: Decay of OAF driven bactericidal activity along the brass tube of the Druett and May (1968) study.

We next consider that the decreasing activity of OAF along the tube was controlled by its loss to the walls. The large flow rate implies turbulent flow conditions (Reynolds number > 30000). If we first assume perfect mixing and interaction of the agent with the wall purely driven by gas kinetics, the observed loss rate coefficient corresponds to an uptake coefficient (γ), the net, fractional efficiency (per collision) of loss from the gas-phase: $\gamma = \frac{k_{\mathrm{OAF}} d}{\omega}$, where ω is the mean thermal velocity of the OAF ‘molecule’. Assuming a molecular weight between 50 and 150 g mole^{-1} and the range for k_{OAF} obtained above, γ is in the range $(1 – 5) \times 10^{-4}$. However, even under highly turbulent conditions, a quasi-stagnant boundary layer persists that effectively limits mass transport and could lead to an effective wall loss rate that is up to two orders of magnitude smaller (Seeley et al., 1996; Seeley et al., 1993; Donahue et al., 1996; Herndon et al., 2001). As this near-surface resistance to uptake cannot be readily assessed retrospectively for the Druett and May experiment, we conservatively conclude that the loss of OAF to the brass walls in the experiment of Druett and May is consistent with an uptake coefficient in the range of 10^{-4} to 10^{-2}.

Peroxides could fit into this range for the wall loss. For example, H_2O_2 is readily destroyed on metal and metal-oxide surfaces, for which a γ value of 1×10^{-4} has been recommended (Crowley et al., 2010). Similar uptake coefficients were observed for peracetic acid (Wu et al., 2015), and also a range of hydroperoxides from isoprene and terpene ozonolysis efficiently partition and react on or in condensed phases (Riva et al., 2017). Peroxy-radicals, with γ values ranging between 10^{-4} and 10^{-2} depending on the substrate (Ammann et al., 2013; Lakey et al., 2015; Lakey et al., 2016) also fit into this range, with higher values obtained in the presence of transition metals that may also be present in a brass tube exposed to acidifying gases. We note that the analysis of Hood (1974) did not consider the possibility that only a fraction of the collisions of the OAF with the wall may lead to its loss, which implies that the molecular weight may be overestimated so that smaller molecules and radicals considered here might remain candidates.

5. MCM Modelling of selected Dark and Nash experiments,

The chamber experiments of Dark and Nash (1970) were reanalysed using a detailed chemical model based on the present version of the Master Chemical Mechanism (MCMv3.2, http://mcm.leeds.ac.uk/MCMv3.2/). Simulations of reactant loss and product formation were performed for six different alkenes (propene, but-1-ene, *trans*-but-2-ene, *cis*-but-2-ene, pent-1-ene and hex-1-ene for an experiment time of 10 minutes. Initial ozone and alkene concentrations and the conditions (T =293 K and RH = 80 %) of the ozonolysis experiments were as given by Dark and Nash (1970). In total, 18 model runs were performed for the six different alkenes and the three different initial O_3 concentrations listed by Dark and Nash (1970). Concentration profiles of HO radicals, HO_2 radicals, hydrogen peroxide (H_2O_2), organic peroxides (ROOHs), aldehydes (RCHOs), alcohols (ROH), carboxylic acids (RC(O)OH) and organic peroxyl radicals (RO_2) were computed (https://chemie.tropos.de/images/Zusatzmaterial/CoxACP2021.zip). Note, groups such as RCHO contain all different aldehydes formed in the specific cases, i.e. for propene (HCHO, CH_3CHO) and for hexane (HCHO, $CH_3(CH_2)_xCHO$ with x = 0,1,2,3). Figure S3 shows the modelled data for the 11 ppbv initial ozone experiments.

To examine possible relationships between the product median concentration levels and the observed bactericidal effects, correlation coefficients and slopes between the two quantities were calculated. However, a greater slope may not necessarily imply a stronger causal relationship because of the underlying variation within the three different ozone concentrations. Similarly, owing to the small number of datapoints, statistical analyses for each specific ozone concentration revealed no clear correlation.

It is highly likely that not only the concentration but also the rate of transfer of a gas-phase product to the aqueous phase (containing the bacteria) play an important role in defining germicidal efficiency. This is manifest in the well-established principle that an efficient air-borne disinfectant must have a very low vapour pressure (Nash, 1951). For this reason, assuming that the germicidal effect of a trace-gas is proportional to its concentration and inversely proportional to p^0, we calculated the ratio (r_p) of the median concentration (expressed as a pressure) and the saturation vapour pressure (p^0) of trace gas product. Values of p^0 were taken from databases (https://chemie.tropos.de/images/Zusatzmaterial/SI_Tables_Cox_et_al.pdf), www.dguv.de/ifa/stoffdatenbank) or calculated (Compernolle et al., 2011). Values of r_p were found to increase at higher ozone conditions (i.e. higher product concentrations) and for the larger olefins.

In order to eliminate the effect of varying the ozone concentration on the relationship between the experimentally derived death fraction $\mathrm{d}f$ ($\mathrm{d}f = (1 - f) \cdot 100$) and r_p, the absolute differences between $\mathrm{d}f$ and r_p for the various ozone concentrations were used; e.g. $\Delta \mathrm{d}f_{11-4} = \mathrm{d}f_{11} - \mathrm{d}f_4$ and $\Delta r_{p,11-4} = r_{p,11} - r_{p,4}$ represents the differences in both parameters for the model run with 11 and 4 ppbv ozone, respectively. In this way, the relationship of the change in the predicted product concentrations (change in the cause) to the change in the observed death fraction (change in the effect) was studied. Figure S4 shows the relationship between Δdf and Δr_p for two inorganic (HO_2, H_2O_2) and two organic (RC(O)OOH, RCHO) trace-gases. While a positive slope is generally observed, the data is very scattered and with the exception of HO_2, the correlation coefficients are < 0.5. All other trace-gases display correlations similar to that of RCHO with correlation coefficients of about 0.1.

The probability that a trace-gas partitioned to the surface region is able to penetrate through the bacterial membrane can be a key factor in determining germicidal effects. Partitioning coefficients such as the octanol-water-coefficient (K_{OW}) are often used as a proxy because the cell membrane permeability is typically linearly proportional to it (Levin et al., 1984). K_{OW} values for all oxidation products were taken from the EPIsuite database or estimated by the KOWWIN v1.67 estimation method (EPA, 2021; US-EPA, 2012). The values obtained (https://chemie.tropos.de/images/Zusatzmaterial/SI_Tables_Cox_et_al.pdf) indicate an increasing value of K_{OW} with increasing carbon chain length. From the values of K_{OW} thus obtained and the modelled concentration of each trace-gas product we calculated f_{KOW}, which is the median simulated concentration (expressed as a partial pressure) of a product multiplied by its value of K_{OW}. As for the analysis using the saturation vapour pressure, f_{KOW} was not strongly correlated with germicidal efficiency.

Possible reasons for the lack of correlation (with the exception of HO_2) between the germicidal efficiency $\Delta \mathrm{d}f$ and the Δr_{p} or Δf_{KOW} of a trace gas may be related to missing chemistry in the MCM mechanism used or in the assumption of a linear relationship between germicidal efficiency and either r_{p} or K_{OW}.

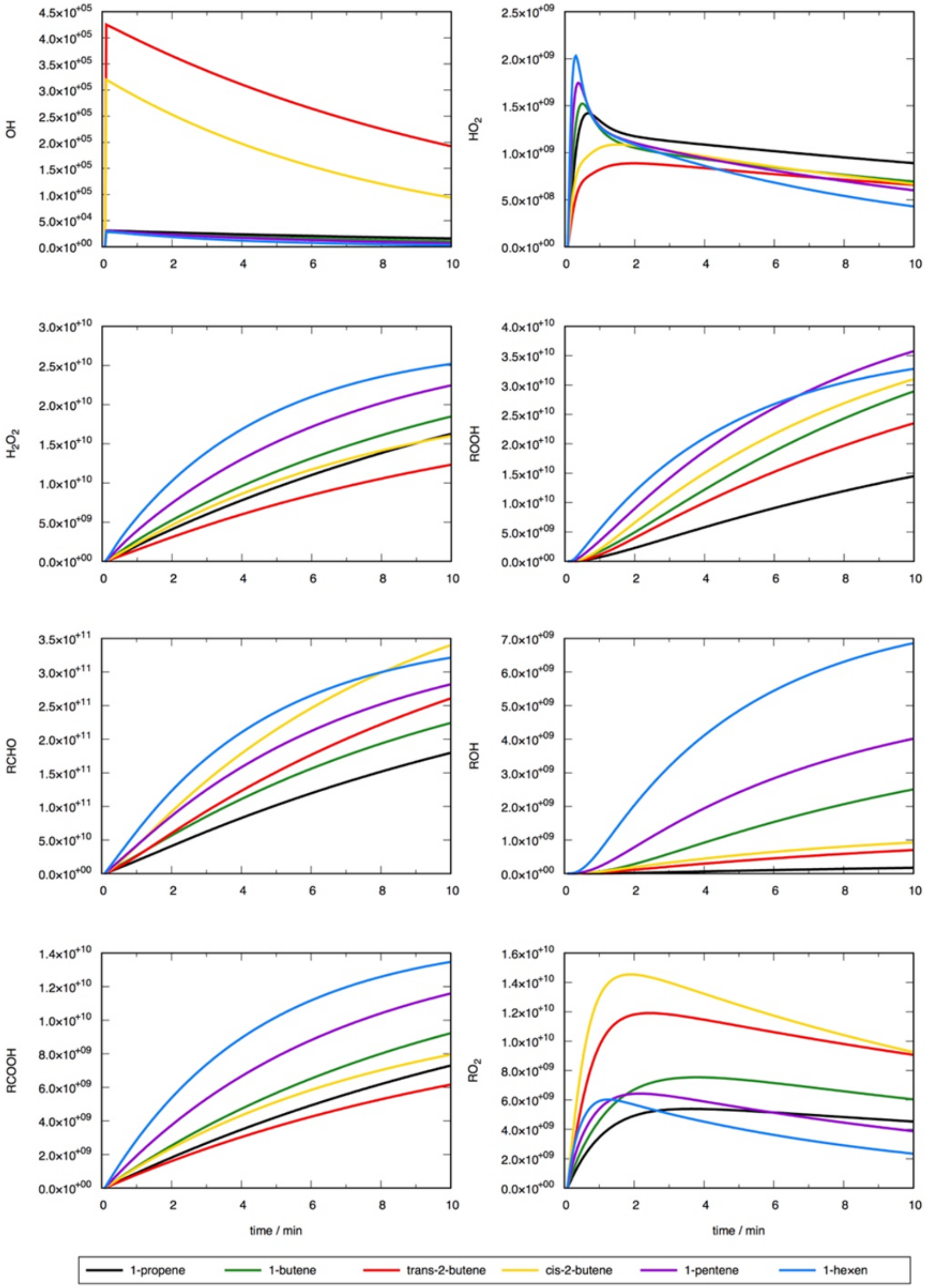


Figure S3: Concentration profiles for HO radicals, HO_2 radicals, H_2O_2, organic hydroperoxides (ROOH), aldehydes (RCHO), alcohols (ROH), carboxylic acids (ROOH), and RO_2 radicals in six different olefin-ozone experiments conducted by Dark and
175 Nash (1970).

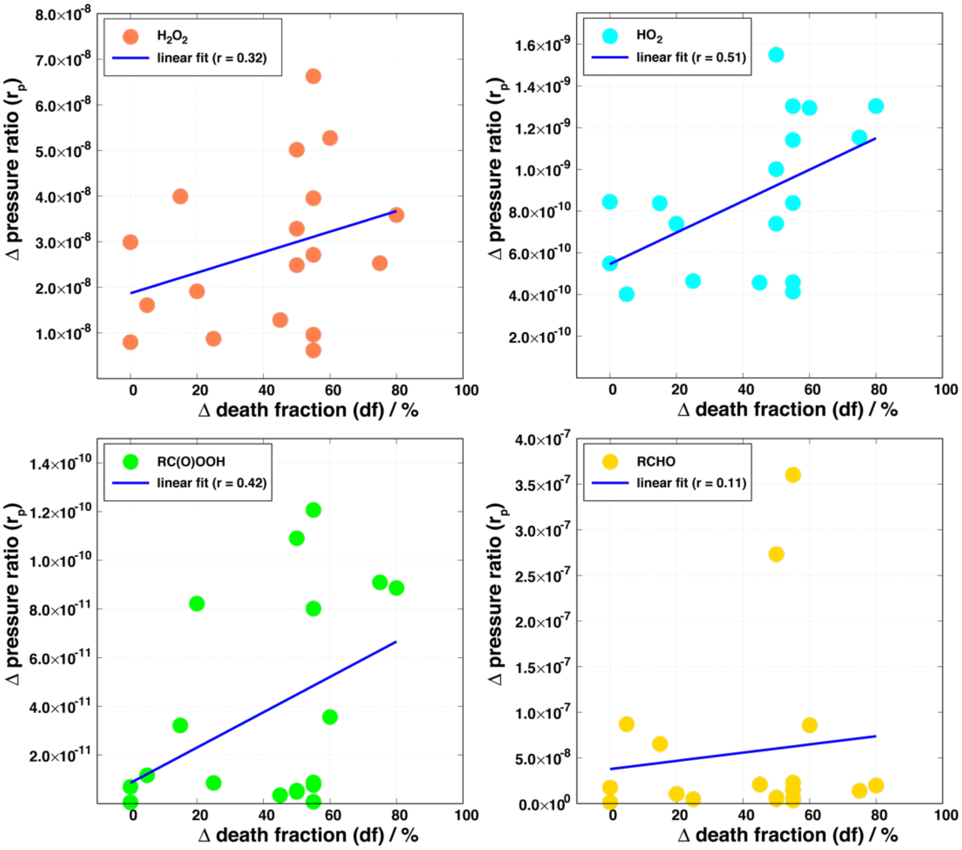


Figure S4: Relationship between the absolute differences of the death fraction (df) of *Escherichia coli* and the calculated r_p ratio of the different model runs for H_2O_2, HO_2, peracids (R(O)OOH) and aldehydes (RCHO).

6. Calculations using updated alkene degradation chemistry

The chemistry of small alkenes, as represented in the MCM, currently is based on the rules defined by Jenkin et al. (Jenkin et al., 1997). To take account of recent advances in understanding, updated chemical schemes were constructed for the 11 alkenes shown in Fig. 1 of the main paper, the ozonolysis of which resulted in the wide range of germicidal impacts reported by Dark and Nash (Dark and Nash, 1970). Importantly, this included chemical schemes for cyclohexene and 2,4,4-trimethypent-2-ene, for which the reported impacts were at the extremes of the range, these alkenes not being treated in the MCM. The new and updated schemes represented explicitly the O_3 and HO-initiated gas-phase chemistry of the series of alkenes to first-generation products under NO_x-free conditions, with the rate coefficients for these initiation reactions taken from Cox et al. (Cox et al., 2020), Mellouki et al. (Mellouki et al., 2021, 2020) and McGillen et al. (McGillen et al., 2020). The schemes included excited Criegee intermediate (CI*) chemistry designed to recreate recommended HO and sCI yields (e.g. as reported by Cox et al.

(Cox et al., 2020)), primary carbonyl yields (e.g. as summarized by Calvert et al. (Calvert et al., 2015) and Cox et al. (Cox et al., 2020)), and reported yields of other products formed from the prompt decomposition of CI* (e.g. HO_2, ketenes, etc.), where available, e.g. Tuazon et al. (Tuazon et al., 1997) for propene, *cis*-but-2-ene, *trans*-but-2-ene and 2-methybut-2-ene; Aschmann et al. (Aschmann et al., 2003) and Hansel et al. (Hansel et al., 2018) for cyclohexene.

The sCI chemistry was based on, or inferred from the recommendations of Cox et al. (2020) and the theoretical/structure-activity relationship (SAR) methods of Vereecken et al. (Vereecken et al., 2017). This includes unimolecular decomposition (e.g. to form HO and organic radical co-products), reaction with H_2O and $(H_2O)_2$, and reaction with the primary carbonyl and carboxylic acid products formed in each alkene system to form secondary ozonides and hydroperoxy-esters.

The bimolecular reactions of peroxy (RO_2) radicals formed from the O_3 and HO-initiated chemistry was based on the recommendations of Jenkin et al. (Jenkin et al., 2019), with a parameterized representation of RO_2 permutation reactions. In the specific case of the complex C_6 RO_2 radicals formed from cyclohexene oxidation, unimolecular isomerization reactions were included, based on the methods of Vereecken and Nozière (Vereecken and Nozière, 2020), allowing rapid formation of HOMs via the resultant autooxidation mechanism, and the formation of the main series of products reported by Aschmann et al. (Aschmann et al., 2003) and Hansel et al. (Hansel et al., 2018). Where appropriate, the decomposition and isomerization chemistry of the oxy (RO) radicals formed in the various systems was based on the methods of Vereecken and Peeters (Vereecken and Peeters, 2010, 2009). The new mechanisms are listed in Table S4, along with a key to species identity in Table S5.

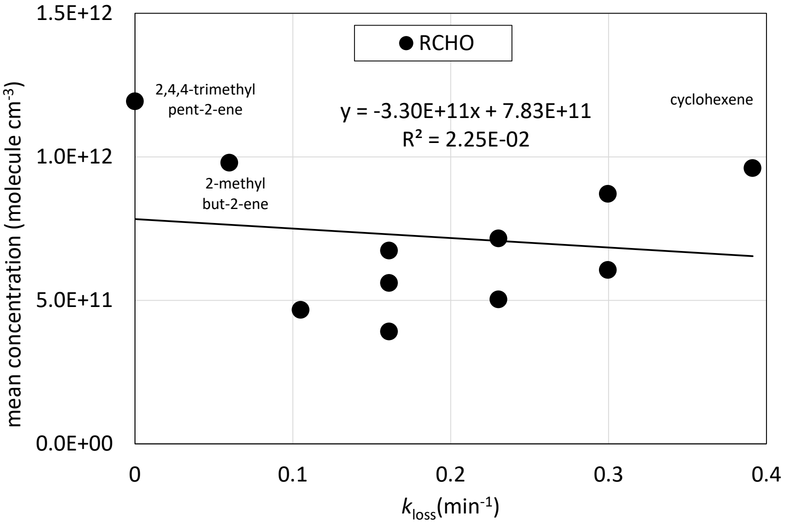


Figure S5: Simulated concentrations of aldehyde products (RCHO) vs. k_{loss} for *E. coli* in 33 ppb O_3 experiments for the series of 11 alkenes shown in Fig. 1 of the main paper; and linear regression of the data.

Simulations of the 11 alkene systems were carried out for each of the three ozone regimes for the 10 minute experiment duration, using the initial conditions reported by Dark and Nash (1970). The average gas-phase concentrations of a series of products or product classes were plotted against the average *E. coli* loss rates (k_{loss}) summarised in Table S1. The products included sCIs, the radical species HO, HO_2 and RO_2, and the closed-shell products, RCHO, RC(O)R, H_2O_2, ROOH, RC(O)OOH, RC(O)OH, ketenes and secondary ozonides. No clear correlations were observed for any product. Figure 2a of the main text shows example results for species containing -OOH groups (including H_2O_2, ROOH and RC(O)OOH) and Fig. S5 the results for RCHO for the 33 ppb ozone experiments. In each case, the concentrations generated from alkenes with low (or zero) germicidal impacts (2-methylbut-2-ene and 2,4,4-trimethylpent-2-ene) are comparable with those generated from cyclohexene, which has the highest germicidal impact.

It is noted, however, that the broad product classes formed in the various systems can include a structurally diverse set of compounds, which may possess different propensities to penetrate the protective membrane of the microorganisms and initiate oxidation. Peroxidic compounds such as H_2O_2 and peracetic acid ($CH_3C(O)OOH$) are known germicides (e.g. (McDonnell and Russell, 1999)), and the speciation was considered in more detail. Figure 2b,c,d of the main text shows the simulated speciation of peroxidic compounds generated from the ozonolysis of 2-methylbut-2-ene, 2,4,4-trimethylpent-2-ene and cyclohexene (33 ppb ozone experiments). For 2-methylbut-2-ene and 2,4,4-trimethylpent-2-ene, the most important contributors are the β-hydroxy species formed from secondary attack of HO on the parent alkenes (accounting of 75 % and 63 % of the peroxide burden, respectively) with additional contributions resulting mainly from the chemistry of the organic co-radical(s) formed with HO from the ozonolysis mechanism (e.g. $CH_3C(O)CH_2OOH$, $CH_3C(O)OOH$ and CH_3OOH from the chemistry of $CH_3C(O)CH_2$ co-radical, and $HC(O)CH_2OOH$ from the chemistry of $HC(O)CH_2$ co-radical in the 2-methylbut-2-ene system). As a result, the peroxide concentrations for the complete series of acyclic alkenes (Fig. S3) broadly follow the trend in HO yields, with underlying contributions from α-hydroxy ROOH and H_2O_2 formed from the reactions of some sCIs with H_2O and $(H_2O)_2$. In the case of cyclohexene, however, important additional contributions result from autooxidation chemistry involving peroxy radicals formed from the organic co-radical, $HC(O)CH_2CH_2CH_2CHCHO$. This leads to additional rapid formation of a number of multi-functional species (HOMs) containing -OOH and -C(O)OOH groups, resulting from sequential H-shift isomerisation reactions, as also reported experimentally (e.g. Hansel et al., 2018). It is probable that such multifunctional species may show an increased propensity for uptake to surfaces. In contrast, it is noted that the majority of hydroperoxide species formed from 2-methylbut-2-ene and 2,4,4-trimethylpent-2-ene are either tertiary and/or contain bulky β-substituents. Clearly further work is required on the structural dependence of germicidal properties of hydroperoxides and other oxygenated products of alkene ozonolysis.

Table S4: Updated chemical schemes for the 11 alkenes shown in Fig. 1 of the main paper. A key to species identity is provided in Table S5.[a]

Rate coefficient [b]	**Reaction**
Propene	
O_3 initiation reactions	
5.77E-15*EXP(-1880/T)*0.35	O3 + C3H6 = CH2OOA + CH3CHO
5.77E-15*EXP(-1880/T)*0.32	O3 + C3H6 = ZCH3CHOOA + HCHO
5.77E-15*EXP(-1880/T)*0.33	O3 + C3H6 = ECH3CHOOA + HCHO
Excited CI chemistry	
KDEC*0.6 [c]	CH2OOA = CH2OO
KDEC*0.118	CH2OOA = CO + HO2 + OH
KDEC*0.124	CH2OOA = CO
KDEC*0.124	CH2OOA = H2
KDEC*0.034	CH2OOA = HO2 + HO2
KDEC*0.13	ZCH3CHOOA = ZCH3CHOO
KDEC*0.87	ZCH3CHOOA = HCOCH2O2 + OH
KDEC*0.13	ECH3CHOOA = ECH3CHOO
KDEC*0.334	ECH3CHOOA = CH4
KDEC*0.192	ECH3CHOOA = CH3OH + CO
KDEC*0.125	ECH3CHOOA = CH2CO
KDEC*0.219	ECH3CHOOA = CH3O2 + HO2
Stabilized sCI chemistry	
2.8E-16*[H_2O]*0.73	CH2OO = HOCH2OOH
2.8E-16*[H_2O]*0.06	CH2OO = HCHO + H2O2
2.8E-16*[H_2O]*0.21	CH2OO = HCOOH
7.35E-18*EXP(4076/T)*[$(H_2O)_2$]*0.40	CH2OO = HOCH2OOH
7.35E-18*EXP(4076/T)*[$(H_2O)_2$]*0.06	CH2OO = HCHO + H2O2
7.35E-18*EXP(4076/T)*[$(H_2O)_2$]*0.54	CH2OO = HCOOH
1.52E-11*EXP(590/T)	CH2OO + HCOOH = HPMEFORM
1.30E-10	CH2OO + CH3CO2H = HPMEACET
1.70E-12	CH2OO + HCHO = CSOZC

1.70E-12	CH2OO + CH3CHO = C2SOZC
7.4E+6*EXP(-3220/T)	ZCH3CHOO = HCOCH2O2 + OH
6.84E-19*$[H_2O]$*0.73	ZCH3CHOO = CH3CHOHOOH
6.84E-19*$[H_2O]$*0.06	ZCH3CHOO = CH3CHO + H2O2
6.84E-19*$[H_2O]$*0.21	ZCH3CHOO = CH3CO2H
2.05E-15*$[(H_2O)_2]$*0.40	ZCH3CHOO = CH3CHOHOOH
2.05E-15*$[(H_2O)_2]$*0.06	ZCH3CHOO = CH3CHO + H2O2
2.05E-15*$[(H_2O)_2]$*0.54	ZCH3CHOO = CH3CO2H
2.50E-10	ZCH3CHOO + HCOOH = HP1ETFORM
1.70E-10	ZCH3CHOO + CH3CO2H = HP1ETACET
1.70E-12	ZCH3CHOO + HCHO = C2SOZC
1.70E-12	ZCH3CHOO + CH3CHO = C2SOZC2
1.94E+09*$T^{1.35}$*EXP(-7445/T)	ECH3CHOO = CH3CO2H
1.3E-14*$[H_2O]$*0.73	ECH3CHOO = CH3CHOHOOH
1.3E-14*$[H_2O]$*0.06	ECH3CHOO = CH3CHO + H2O2
1.3E-14*$[H_2O]$*0.21	ECH3CHOO = CH3CO2H
4.4E-11*$[(H_2O)_2]$*0.40	ECH3CHOO = CH3CHOHOOH
4.4E-11*$[(H_2O)_2]$*0.06	ECH3CHOO = CH3CHO + H2O2
4.4E-11*$[(H_2O)_2]$*0.54	ECH3CHOO = CH3CO2H
5.00E-10	ECH3CHOO + HCOOH = HP1ETFORM
2.50E-10	ECH3CHOO + CH3CO2H = HP1ETACET
1.70E-12	ECH3CHOO + HCHO = C2SOZC
1.70E-12	ECH3CHOO + CH3CHO = C2SOZC2
OH initiation reactions	
KMT16*0.137 [d]	OH + C3H6 = HYPROPO2
KMT16*0.863	OH + C3H6 = IPROPOLO2
RO_2 and RO chemistry	
KRO2HO2*0.498*0.82 [e]	HCOCH2O2 + HO2 = HCOCH2OOH
KRO2HO2*0.498*0.18	HCOCH2O2 + HO2 = HCOCH2O + OH
1.00E-13*EXP(974/T)*0.2*$[RO_2]$ [f]	HCOCH2O2 = GLYOX
1.00E-13*EXP(974/T)*0.6*$[RO_2]$	HCOCH2O2 = HCOCH2O
1.00E-13*EXP(974/T)*0.2*$[RO_2]$	HCOCH2O2 = HOCH2CHO

KDEC	HCOCH2O = HCHO + CO + HO2
3.8E-13*EXP(780/T)*(1-1/(1+498*EXP(-1160/T)))	CH3O2 + HO2 = CH3OOH
3.8E-13*EXP(780/T)*(1/(1+498*EXP(-1160/T)))	CH3O2 + HO2 = HCHO
2.06E-13*EXP(365/T)*7.2*EXP(-885/T)*$[RO_2]$	CH3O2 = CH3O
1.03E-13*EXP(365/T)*(1-7.2*EXP(-885/T))*$[RO_2]$	CH3O2 = CH3OH
1.03E-13*EXP(365/T)*(1-7.2*EXP(-885/T))*$[RO_2]$	CH3O2 = HCHO
7.2E-14*EXP(-1080/T)*$[O_2]$	CH3O = HCHO + HO2
KRO2HO2*0.601	HYPROPO2 + HO2 = HYPROPO2H
1.00E-13*EXP(570/T)*0.2*$[RO_2]$	HYPROPO2 = ACETOL
1.00E-13*EXP(570/T)*0.6*$[RO_2]$	HYPROPO2 = HYPROPO
1.00E-13*EXP(570/T)*0.2*$[RO_2]$	HYPROPO2 = PROPGLY
2.00E+14*EXP(-6410/T)	HYPROPO = CH3CHO + HCHO + HO2
KRO2HO2*0.601	IPROPOLO2 + HO2 = IPROPOLO2H
1.00E-13*EXP(942/T)*0.2*$[RO_2]$	IPROPOLO2 = CH3CHOHCHO
1.00E-13*EXP(942/T)*0.6*$[RO_2]$	IPROPOLO2 = IPROPOLO
1.00E-13*EXP(942/T)*0.2*$[RO_2]$	IPROPOLO2 = PROPGLY
2.00E+14*EXP(-5505/T)	IPROPOLO = CH3CHO + HCHO + HO2
But-1-ene	
O_3 initiation reactions	
3.55E-15*EXP(-1750/T)*0.35	O3 + BUT1ENE = CH2OOB + C2H5CHO
3.55E-15*EXP(-1750/T)*0.325	O3 + BUT1ENE = ZC2H5CHOOA + HCHO
3.55E-15*EXP(-1750/T)*0.325	O3 + BUT1ENE = EC2H5CHOOA + HCHO
Excited CI chemistry	
KDEC*0.7	CH2OOB = CH2OO
KDEC*0.088	CH2OOB = CO + HO2 + OH
KDEC*0.093	CH2OOB = CO
KDEC*0.093	CH2OOB = H2
KDEC*0.026	CH2OOB = HO2 + HO2
KDEC*0.15	ZC2H5CHOOA = ZC2H5CHOO
KDEC*0.85	ZC2H5CHOOA = PROPALO2 + OH
KDEC*0.15	EC2H5CHOOA = EC2H5CHOO

KDEC*0.326	EC2H5CHOOA = C2H6
KDEC*0.188	EC2H5CHOOA = C2H5OH + CO
KDEC*0.122	EC2H5CHOOA = CH3CHCO
KDEC*0.214	EC2H5CHOOA = C2H5O2 + HO2
Stabilized sCI chemistry	
1.30E-10	CH2OO + PROPACID = HPMEPROP
1.70E-12	CH2OO + C2H5CHO = C3SOZC
2.41E-62*$T^{24.33}$*EXP(2571/T)	ZC2H5CHOO = PROPALO2 + OH
1.51E-18*[H_2O]*0.73	ZC2H5CHOO = ETCHOHOOH
1.51E-18*[H_2O]*0.06	ZC2H5CHOO = C2H5CHO + H2O2
1.51E-18*[H_2O]*0.21	ZC2H5CHOO = PROPACID
4.31E-15*[$(H_2O)_2$]*0.40	ZC2H5CHOO = ETCHOHOOH
4.31E-15*[$(H_2O)_2$]*0.06	ZC2H5CHOO = C2H5CHO + H2O2
4.31E-15*[$(H_2O)_2$]*0.54	ZC2H5CHOO = PROPACID
2.50E-10	ZC2H5CHOO + HCOOH = HP1PRFORM
1.70E-10	ZC2H5CHOO + PROPACID = HP1PRPROP
1.70E-12	ZC2H5CHOO + HCHO = C3SOZC
1.70E-12	ZC2H5CHOO + C2H5CHO = C3SOZC3
1.57E10*$T^{1.03}$*EXP(-7464/T)	EC2H5CHOO = PROPACID
1.58E-14*[H_2O]*0.73	EC2H5CHOO = ETCHOHOOH
1.58E-14*[H_2O]*0.06	EC2H5CHOO = C2H5CHO + H2O2
1.58E-14*[H_2O]*0.21	EC2H5CHOO = PROPACID
1.75E-11*[$(H_2O)_2$]*0.40	EC2H5CHOO = ETCHOHOOH
1.75E-11*[$(H_2O)_2$]*0.06	EC2H5CHOO = C2H5CHO + H2O2
1.75E-11*[$(H_2O)_2$]*0.54	EC2H5CHOO = PROPACID
5.00E-10	EC2H5CHOO + HCOOH = HP1PRFORM
2.50E-10	EC2H5CHOO + PROPACID = HP1PRPROP
1.70E-12	EC2H5CHOO + HCHO = C3SOZC
1.70E-12	EC2H5CHOO + C2H5CHO = C3SOZC3
OH initiation reactions	
6.6E-12*EXP(465/T)*0.137	BUT1ENE + OH = HO3C4O2
6.6E-12*EXP(465/T)*0.863	BUT1ENE + OH = NBUTOLAO2

RO_2 and RO chemistry	
6.4E-13*EXP(710/T)	C2H5O2 + HO2 = C2H5OOH
1.00E-13*EXP(353/T)*0.6*[RO_2]	C2H5O2 = C2H5O
1.00E-13*EXP(353/T)*0.2*[RO_2]	C2H5O2 = C2H5OH
1.00E-13*EXP(353/T)*0.2*[RO_2]	C2H5O2 = CH3CHO
2.4E-14*EXP(-325/T)*[O_2]	C2H5O = CH3CHO + HO2
KRO2HO2*0.601*0.82	PROPALO2 + HO2 = PROPALOOH
KRO2HO2*0.601*0.18	PROPALO2 + HO2 = PROPALO + OH
1.00E-13*EXP(674/T)*0.2*[RO_2]	PROPALO2 = CH3CHOHCHO
1.00E-13*EXP(674/T)*0.2*[RO_2]	PROPALO2 = MGLYOX
1.00E-13*EXP(674/T)*0.6*[RO_2]	PROPALO2 = PROPALO
KDEC	PROPALO = CH3CHO + HO2 + CO
KRO2HO2*0.683	HO3C4O2 + HO2 = HO3C4OOH
1.00E-13*EXP(983/T)*0.2*[RO_2]	HO3C4O2 = HO3C3CHO
1.00E-13*EXP(983/T)*0.6*[RO_2]	HO3C4O2 = HO3C4O
1.00E-13*EXP(983/T)*0.2*[RO_2]	HO3C4O2 = NBUTOLAOH
1.80E+13*EXP(-5234/T)	HO3C4O = C2H5CHO + HCHO + HO2
1.20E+11*EXP(-3825/T)	HO3C4O = HO34C4O2
KRO2HO2*0.683	NBUTOLAO2 + HO2 = NBUTOLAOOH
1.00E-13*EXP(675/T)*0.2*[RO_2]	NBUTOLAO2 = MEKCOH
1.00E-13*EXP(675/T)*0.6*[RO_2]	NBUTOLAO2 = NBUTOLAO
1.00E-13*EXP(675/T)*0.2*[RO_2]	NBUTOLAO2 = NBUTOLAOH
2.00E+14*EXP(-6354/T)	NBUTOLAO = C2H5CHO + HCHO + HO2
KRO2HO2*0.748	HO34C4O2 + HO2 = HO34C4OOH
1.00E-13*EXP(785/T)*0.2*[RO_2]	HO34C4O2 = HO34C3CHO
1.00E-13*EXP(785/T)*0.6*[RO_2]	HO34C4O2 = HO34C4O
1.00E-13*EXP(785/T)*0.2*[RO_2]	HO34C4O2 = HO13C4OH
8.00E+10*EXP(-2417/T)	HO34C4O = HO13C3CHO + HO2
Pent-1-ene	
O_3 initiation reactions	
2.13E-15*EXP(-1580/T)*0.35	PENT1ENE + O3 = CH2OOC + C3H7CHO
2.13E-15*EXP(-1580/T)*0.325	PENT1ENE + O3 = ZC3H7CHOOA + HCHO

2.13E-15*EXP(-1580/T)*0.325	PENT1ENE + O3 = EC3H7CHOOA + HCHO
Excited CI chemistry	
KDEC*0.9	CH2OOC = CH2OO
KDEC*0.029	CH2OOC = CO + HO2 + OH
KDEC*0.031	CH2OOC = CO
KDEC*0.031	CH2OOC = H2
KDEC*0.009	CH2OOC = HO2 + HO2
KDEC*0.19	ZC3H7CHOOA = ZC3H7CHOO
KDEC*0.81	ZC3H7CHOOA = BUTALAO2 + OH
KDEC*0.19	EC3H7CHOOA = EC3H7CHOO
KDEC*0.311	EC3H7CHOOA = C3H8
KDEC*0.179	EC3H7CHOOA = NPROPOL + CO
KDEC*0.116	EC3H7CHOOA = C2H5CHCO
KDEC*0.204	EC3H7CHOOA = NC3H7O2 + HO2
Stabilized sCI chemistry	
1.30E-10	CH2OO + BUTACID = HPMEBUTR
1.70E-12	CH2OO + C3H7CHO = C4SOZC
2.41E-62*$T^{24.33}$*EXP(2571/T)	ZC3H7CHOO = BUTALAO2 + OH
1.51E-18*$[H_2O]$*0.73	ZC3H7CHOO = PRCHOHOOH
1.51E-18*$[H_2O]$*0.06	ZC3H7CHOO = C3H7CHO + H2O2
1.51E-18*$[H_2O]$*0.21	ZC3H7CHOO = BUTACID
4.31E-15*$[(H_2O)_2]$*0.40	ZC3H7CHOO = PRCHOHOOH
4.31E-15*$[(H_2O)_2]$*0.06	ZC3H7CHOO = C3H7CHO + H2O2
4.31E-15*$[(H_2O)_2]$*0.54	ZC2H5CHOO = BUTACID
2.50E-10	ZC3H7CHOO + HCOOH = HP1BUFORM
1.70E-10	ZC3H7CHOO + BUTACID = HP1BUBUTR
1.70E-12	ZC3H7CHOO + HCHO = C4SOZC
1.70E-12	ZC3H7CHOO + C3H7CHO = C4SOZC4
1.57E10*$T^{1.03}$*EXP(-7464/T)	EC3H7CHOO = BUTACID
1.58E-14*$[H_2O]$*0.73	EC3H7CHOO = PRCHOHOOH
1.58E-14*$[H_2O]$*0.06	EC3H7CHOO = C3H7CHO + H2O2

1.58E-14*[H_2O]*0.21	EC3H7CHOO = BUTACID
1.75E-11*[$(H_2O)_2$]*0.40	EC3H7CHOO = PRCHOHOOH
1.75E-11*[$(H_2O)_2$]*0.06	EC3H7CHOO = C3H7CHO + H2O2
1.75E-11*[$(H_2O)_2$]*0.54	EC3H7CHOO = BUTACID
5.00E-10	EC3H7CHOO + HCOOH = HP1BUFORM
2.50E-10	EC3H7CHOO + BUTACID = HP1BUBUTR
1.70E-12	EC3H7CHOO + HCHO = C4SOZC
1.70E-12	EC3H7CHOO + C3H7CHO = C4SOZC4
OH initiation reactions	
5.86E-12*EXP(500/T)*0.863	PENT1ENE + OH = PE1ENEAO2
5.86E-12*EXP(500/T)*0.137	PENT1ENE + OH = PE1ENEBO2
RO_2 and RO chemistry	
KRO2HO2*0.498	NC3H7O2 + HO2 = NC3H7OOH
1.00E-13*EXP(559/T)*0.2*[RO_2]	NC3H7O2 = C2H5CHO
1.00E-13*EXP(559/T)*0.6*[RO_2]	NC3H7O2 = NC3H7O
1.00E-13*EXP(559/T)*0.2*[RO_2]	NC3H7O2 = NPROPOL
2.6E-14*EXP(-255/T)*[O_2]	NC3H7O = C2H5CHO + HO2
KRO2HO2*0.683*0.82	BUTALAO2 + HO2 = BUTALAOOH
KRO2HO2*0.683*0.18	BUTALAO2 + HO2 = BUTAL2O + OH
1.00E-13*EXP(779/T)*0.6*[RO_2]	BUTALAO2 = BUTAL2O
1.00E-13*EXP(779/T)*0.2*[RO_2]	BUTALAO2 = EGLYOX
1.00E-13*EXP(779/T)*0.2*[RO_2]	BUTALAO2 = HO3C3CHO
KDEC	BUTAL2O = C2H5CHO + HO2 + CO
KRO2HO2*0.748	PE1ENEAO2 + HO2 = C51OH2OOH
1.00E-13*EXP(731/T)*0.2*[RO_2]	PE1ENEAO2 = C51OH2CO
1.00E-13*EXP(731/T)*0.2*[RO_2]	PE1ENEAO2 = HO12C5
1.00E-13*EXP(731/T)*0.6*[RO_2]	PE1ENEAO2 = PE1ENEAO
1.80E+13*EXP(-4076/T)	PE1ENEAO = C3H7CHO + HCHO + HO2
KRO2HO2*0.748	PE1ENEBO2 + HO2 = C52OH1OOH
1.00E-13*EXP(1007/T)*0.2*[RO_2]	PE1ENEBO2 = C4OHCHO
1.00E-13*EXP(1007/T)*0.2*[RO_2]	PE1ENEBO2 = HO12C5
1.00E-13*EXP(1007/T)*0.6*[RO_2]	PE1ENEBO2 = PE1ENEBO

1.80E+13*EXP(-5234/T)	PE1ENEBO = C3H7CHO + HCHO + HO2
8.00E+10*EXP(-3010/T)	PE1ENEBO = HO12C54O2
KRO2HO2*0.800	HO12C54O2 + HO2 = HO12C54OOH
1.00E-13*EXP(373/T)*0.2*[RO_2]	HO12C54O2 = C51OH
1.00E-13*EXP(373/T)*0.2*[RO_2]	HO12C54O2 = HO124C5
1.00E-13*EXP(373/T)*0.6*[RO_2]	HO12C54O2 = HO12C54O
8.00E+10*EXP(-2417/T)	HO12C54O = HO24C4CHO + HO2
Hex-1-ene	
O_3 initiation reactions	
1.33E-15*EXP(-1480/T)*0.35	HEX1ENE + O3 = CH2OO + C4H9CHO
1.33E-15*EXP(-1480/T)*0.325	HEX1ENE + O3 = HCHO + ZC4H9CHOOA
1.33E-15*EXP(-1480/T)*0.325	HEX1ENE + O3 = HCHO + EC4H9CHOOA
Excited CI chemistry	
KDEC*0.25	ZC4H9CHOOA = ZC4H9CHOO
KDEC*0.75	ZC4H9CHOOA = C4CHOAO2 + OH
KDEC*0.25	EC4H9CHOOA = EC4H9CHOO
KDEC*0.288	EC4H9CHOOA = NC4H10
KDEC*0.166	EC4H9CHOOA = NBUTOL + CO
KDEC*0.107	EC4H9CHOOA = C3H7CHCO
KDEC*0.189	EC4H9CHOOA = NC4H9O2 + HO2
Stabilized sCI chemistry	
1.30E-10	CH2OO + PENTACID = HPMEPENT
1.70E-12	CH2OO + C4H9CHO = C5SOZC
2.41E-62*$T^{24.33}$*EXP(2571/T)	ZC4H9CHOO = C4CHOAO2 + OH
1.51E-18*[H_2O]*0.73	ZC4H9CHOO = BUCHOHOOH
1.51E-18*[H_2O]*0.06	ZC4H9CHOO = C4H9CHO + H2O2
1.51E-18*[H_2O]*0.21	ZC4H9CHOO = PENTACID
4.31E-15*[$(H_2O)_2$]*0.40	ZC4H9CHOO = BUCHOHOOH
4.31E-15*[$(H_2O)_2$]*0.06	ZC4H9CHOO = C4H9CHO + H2O2
4.31E-15*[$(H_2O)_2$]*0.54	ZC4H9CHOO = PENTACID
2.50E-10	ZC4H9CHOO + HCOOH = HP1PEFORM

1.70E-10	ZC4H9CHOO + PENTACID = HP1PEPENT
1.70E-12	ZC4H9CHOO + HCHO = C5SOZC
1.70E-12	ZC4H9CHOO + C4H9CHO = C5SOZC5
1.57E10*$T^{1.03}$*EXP(-7464/T)	EC4H9CHOO = PENTACID
1.58E-14*[H_2O]*0.73	EC4H9CHOO = BUCHOHOOH
1.58E-14*[H_2O]*0.06	EC4H9CHOO = C4H9CHO + H2O2
1.58E-14*[H_2O]*0.21	EC4H9CHOO = PENTACID
1.75E-11*[$(H_2O)_2$]*0.40	EC4H9CHOO = BUCHOHOOH
1.75E-11*[$(H_2O)_2$]*0.06	EC4H9CHOO = C4H9CHO + H2O2
1.75E-11*[$(H_2O)_2$]*0.54	EC4H9CHOO = PENTACID
5.00E-10	EC4H9CHOO + HCOOH = HP1PEFORM
2.50E-10	EC4H9CHOO + PENTACID = HP1PEPENT
1.70E-12	EC4H9CHOO + HCHO = C5SOZC
1.70E-12	EC4H9CHOO + C4H9CHO = C5SOZC5
OH initiation reactions	
3.70E-11*0.863	HEX1ENE + OH = C6OH5O2
3.70E-11*0.137	HEX1ENE + OH = HO5C6O2
RO_2 and RO chemistry	
KRO2HO2*0.601	NC4H9O2 + HO2 = NC4H9OOH
1.00E-13*EXP(667/T)*0.2*[RO_2]	NC4H9O2 = C3H7CHO
1.00E-13*EXP(667/T)*0.2*[RO_2]	NC4H9O2 = NBUTOL
1.00E-13*EXP(667/T)*0.6*[RO_2]	NC4H9O2 = NC4H9O
8.9E-14*EXP(-550/T)*[O_2]	NC4H9O = C3H7CHO + HO2
4.6D10*EXP(-3570/T)	NC4H9O = HO1C4O2
KRO2HO2*0.683	HO1C4O2 + HO2 = HO1C4OOH
1.00E-13*EXP(746/T)*0.6*[RO_2]	HO1C4O2 = HO1C4O
1.00E-13*EXP(746/T)*0.2*[RO_2]	HO1C4O2 = HOC3H6CHO
1.00E-13*EXP(746/T)*0.2*[RO_2]	HO1C4O2 = HOC4H8OH
8.74E+11*EXP(-3430/T)	HO1C4O = HOC3H6CHO + HO2
KRO2HO2*0.748*0.82	C4CHOAO2 + HO2 = C4CHOAOOH
KRO2HO2*0.748*0.18	C4CHOAO2 + HO2 = C4CHO2O + OH
1.00E-13*EXP(834/T)*0.6*[RO_2]	C4CHOAO2 = C4CHO2O

1.00E-13*EXP(834/T)*0.2*[RO_2]	C4CHOAO2 = C4OHCHO
1.00E-13*EXP(834/T)*0.2*[RO_2]	C4CHOAO2 = PGLYOX
KDEC	C4CHO2O = C3H7CHO + HO2 + CO
KRO2HO2*0.800	C6OH5O2 + HO2 = C6OH5OOH
1.00E-13*EXP(760/T)*0.2*[RO_2]	C6OH5O2 = C4COMEOH
1.00E-13*EXP(760/T)*0.2*[RO_2]	C6OH5O2 = C656OH
1.00E-13*EXP(760/T)*0.6*[RO_2]	C6OH5O2 = C6OH5O
1.80E+13*EXP(-4076/T)	C6OH5O = C4H9CHO + HCHO + HO2
8.00E+10*EXP(-3010/T)	C6OH5O = HO12C65O2
KRO2HO2*0.800	HO5C6O2 + HO2 = HO5C6OOH
1.00E-13*EXP(1021/T)*0.2*[RO_2]	HO5C6O2 = C656OH
1.00E-13*EXP(1021/T)*0.2*[RO_2]	HO5C6O2 = HO5C5CHO
1.00E-13*EXP(1021/T)*0.6*[RO_2]	HO5C6O2 = HO5C6O
1.80E+13*EXP(-5234/T)	HO5C6O = HCHO + C4H9CHO + HO2
8.00E+10*EXP(-3010/T)	HO5C6O = HO12C64O2
KRO2HO2*0.841	HO12C65O2 + HO2 = HO12C65OOH
1.00E-13*EXP(399/T)*0.2*[RO_2]	HO12C65O2 = HO12C65CO
1.00E-13*EXP(399/T)*0.2*[RO_2]	HO12C65O2 = HO125C6
1.00E-13*EXP(399/T)*0.6*[RO_2]	HO12C65O2 = HO12C65O
4.00E+10*EXP(-1871/T)	HO12C65O = HO15C62CO + HO2
KRO2HO2*0.841	HO12C64O2 + HO2 = HO12C64OOH
1.00E-13*EXP(399/T)*0.2*[RO_2]	HO12C64O2 = HO12C64CO
1.00E-13*EXP(399/T)*0.2*[RO_2]	HO12C64O2 = HO124C6
1.00E-13*EXP(399/T)*0.6*[RO_2]	HO12C64O2 = HO12C64O
8.00E+10*EXP(-2417/T)	HO12C64O = HO35C5CHO + HO2
cis-But-2-ene	
O_3 initiation reactions	
3.37E-15*EXP(-970/T)*0.33	CBUT2ENE + O3 = CH3CHO + ZCH3CHOOB
3.37E-15*EXP(-970/T)*0.67	CBUT2ENE + O3 = CH3CHO + ECH3CHOOB
Excited CI chemistry	
KDEC*0.50	ZCH3CHOOB = ZCH3CHOO
KDEC*0.50	ZCH3CHOOB = HCOCH2O2 + OH

KDEC*0.32	ECH3CHOOB = ECH3CHOO
KDEC*0.268	ECH3CHOOB = CH4
KDEC*0.138	ECH3CHOOB = CH3OH + CO
KDEC*0.104	ECH3CHOOB = CH2CO
KDEC*0.170	ECH3CHOOB = CH3O2 + HO2
OH initiation reactions	
1.10E-11*EXP(487/T)	CBUT2ENE + OH = BUT2OLO2
RO_2 and RO chemistry	
KRO2HO2*0.683	BUT2OLO2 + HO2 = BUT2OLOOH
1.00E-13*EXP(675/T)*0.6*$[RO_2]$	BUT2OLO2 = BUT2OLAO
1.00E-13*EXP(675/T)*0.2*$[RO_2]$	BUT2OLO2 = BUT2OLO
1.00E-13*EXP(675/T)*0.2*$[RO_2]$	BUT2OLO2 = BUT2OLOH
1.80E+13*EXP(-2528/T)	BUT2OLAO = CH3CHO + CH3CHO + HO2
trans-But-2-ene	
O_3 initiation reactions	
6.64E-15*EXP(-1059/T)*0.6	TBUT2ENE + O3 = CH3CHO + ZCH3CHOOB
6.64E-15*EXP(-1059/T)*0.4	TBUT2ENE + O3 = CH3CHO + ECH3CHOOC
Excited CI chemistry	
KDEC*0.32	ECH3CHOOC = ECH3CHOO
KDEC*0.288	ECH3CHOOC = CH4
KDEC*0.175	ECH3CHOOC = CH3OH + CO
KDEC*0.115	ECH3CHOOC = CH2CO
KDEC*0.102	ECH3CHOOC = CH3O2 + HO2
OH initiation reactions	
1.01E-11*EXP(550/T)	TBUT2ENE + OH = BUT2OLO2
trans-Pent-2-ene	
O_3 initiation reactions	
7.10E-15*EXP(-1132/T)*0.25	TPENT2ENE + O3 = ZC2H5CHOOB + CH3CHO
7.10E-15*EXP(-1132/T)*0.25	TPENT2ENE + O3 = EC2H5CHOOB + CH3CHO
7.10E-15*EXP(-1132/T)*0.25	TPENT2ENE + O3 = ZCH3CHOOC + C2H5CHO
7.10E-15*EXP(-1132/T)*0.25	TPENT2ENE + O3 = ECH3CHOOD + C2H5CHO

Excited CI chemistry	
KDEC*0.58	ZCH3CHOOC = ZCH3CHOO
KDEC*0.42	ZCH3CHOOC = HCOCH2O2 + OH
KDEC*0.58	ECH3CHOOD = ECH3CHOO
KDEC*0.178	ECH3CHOOD = CH4
KDEC*0.108	ECH3CHOOD = CH3OH + CO
KDEC*0.071	ECH3CHOOD = CH2CO
KDEC*0.063	ECH3CHOOD = CH3O2 + HO2
KDEC*0.45	ZC2H5CHOOB = ZC2H5CHOO
KDEC*0.55	ZC2H5CHOOB = PROPALO2 + OH
KDEC*0.45	EC2H5CHOOB = EC2H5CHOO
KDEC*0.233	EC2H5CHOOB = C2H6
KDEC*0.141	EC2H5CHOOB = C2H5OH + CO
KDEC*0.093	EC2H5CHOOB = CH3CHCO
KDEC*0.083	EC2H5CHOOB = C2H5O2 + HO2
Stabilized sCI chemistry	
1.70E-10	ZCH3CHOO + PROPACID = HP1ETPROP
1.70E-12	ZCH3CHOO + C2H5CHO = C3SOZC2
2.50E-10	ECH3CHOO + PROPACID = HP1ETPROP
1.70E-12	ECH3CHOO + C2H5CHO = C3SOZC2
1.70E-10	ZC2H5CHOO + CH3CO2H = HP1PRACET
1.70E-12	ZC2H5CHOO + CH3CHO = C3SOZC2
2.50E-10	EC2H5CHOO + CH3CO2H = HP1PRACET
1.70E-12	EC2H5CHOO + CH3CHO = C3SOZC2
OH initiation reactions	
6.69E-11*0.5	TPENT2ENE + OH = PE2ENEAO2
6.69E-11*0.5	TPENT2ENE + OH = PE2ENEBO2

RO_2 and RO chemistry	
KRO2HO2*0.748	PE2ENEAO2 + HO2 = C52OH3OOH
1.00E-13*EXP(731/T)*0.2*$[RO_2]$	PE2ENEAO2 = C523OH
1.00E-13*EXP(731/T)*0.2*$[RO_2]$	PE2ENEAO2 = DIEKAOH
1.00E-13*EXP(731/T)*0.6*$[RO_2]$	PE2ENEAO2 = PE2ENEAO
1.80E+13*EXP(-2528/T)	PE2ENEAO = C2H5CHO + CH3CHO + HO2
KRO2HO2*0.748	PE2ENEBO2 + HO2 = C53OH2OOH
1.00E-13*EXP(731/T)*0.2*$[RO_2]$	PE2ENEBO2 = C523OH
1.00E-13*EXP(731/T)*0.2*$[RO_2]$	PE2ENEBO2 = MPRKAOH
1.00E-13*EXP(731/T)*0.6*$[RO_2]$	PE2ENEBO2 = PE2ENEBO
1.80E+13*EXP(-2528/T)	PE2ENEBO = CH3CHO + C2H5CHO + HO2
trans-Hex-2-ene	
O_3 initiation reactions	
7.60E-15*EXP(-1163/T)*0.25	THEX2ENE + O3 = C3H7CHO + ZCH3CHOOD
7.60E-15*EXP(-1163/T)*0.25	THEX2ENE + O3 = C3H7CHO + ECH3CHOOE
7.60E-15*EXP(-1163/T)*0.25	THEX2ENE + O3 = CH3CHO + ZC3H7CHOOB
7.60E-15*EXP(-1163/T)*0.25	THEX2ENE + O3 = CH3CHO + EC3H7CHOOB
Excited CI chemistry	
KDEC*0.80	ZCH3CHOOD = ZCH3CHOO
KDEC*0.20	ZCH3CHOOD = HCOCH2O2 + OH
KDEC*0.80	ECH3CHOOE = ECH3CHOO
KDEC*0.085	ECH3CHOOE = CH4
KDEC*0.051	ECH3CHOOE = CH3OH + CO
KDEC*0.034	ECH3CHOOE = CH2CO
KDEC*0.030	ECH3CHOOE = CH3O2 + HO2
KDEC*0.40	ZC3H7CHOOB = ZC3H7CHOO
KDEC*0.60	ZC3H7CHOOB = BUTALAO2 + OH
KDEC*0.40	EC3H7CHOOB = ECH3CHOO
KDEC*0.254	EC3H7CHOOB = C3H8
KDEC*0.155	EC3H7CHOOB = NPROPOL + CO
KDEC*0.101	EC3H7CHOOB = C2H5CHCO
KDEC*0.090	EC3H7CHOOB = NC3H7O2 + HO2

Stabilized sCI chemistry	
1.70E-10	ZCH3CHOO + BUTACID = HP1ETBUTR
1.70E-12	ZCH3CHOO + C3H7CHO = C4SOZC2
2.50E-10	ECH3CHOO + BUTACID = HP1ETBUTR
1.70E-12	ECH3CHOO + C3H7CHO = C4SOZC2
1.70E-10	ZC3H7CHOO + CH3CO2H = HP1BUACET
1.70E-12	ZC3H7CHOO + CH3CHO = C4SOZC2
2.50E-10	EC3H7CHOO + CH3CO2H = HP1BUACET
1.70E-12	EC3H7CHOO + CH3CHO = C4SOZC2
OH initiation reactions	
6.00E-11*0.5	THEX2ENE + OH = C64OH5O2
6.00E-11*0.5	THEX2ENE + OH = C65OH4O2
RO$_2$ and RO chemistry	
KRO2HO2*0.800	C64OH5O2 + HO2 = C64OH5OOH
1.00E-13*EXP(760/T)*0.2*[RO$_2$]	C64OH5O2 = C645OH
1.00E-13*EXP(760/T)*0.6*[RO$_2$]	C64OH5O2 = C64OH5O
1.00E-13*EXP(760/T)*0.2*[RO$_2$]	C64OH5O2 = CO2HO3C6
1.80E+13*EXP(-2528/T)	C64OH5O = CH3CHO + C3H7CHO + HO2
KRO2HO2*0.800	C65OH4O2 + HO2 = C65OH4OOH
1.00E-13*EXP(760/T)*0.2*[RO$_2$]	C65OH4O2 = C645OH
1.00E-13*EXP(760/T)*0.6*[RO$_2$]	C65OH4O2 = C65OH4O
1.00E-13*EXP(760/T)*0.2*[RO$_2$]	C65OH4O2 = HEX3ONCOH
1.80E+13*EXP(-2528/T)	C65OH4O = C3H7CHO + CH3CHO + HO2
2-Methyl-but-2-ene	
O$_3$ initiation reactions	
6.51E-15*EXP(-829/T)*0.63	ME2BUT2ENE + O3= CH3CHO + CH3CCH3OOA
6.51E-15*EXP(-829/T)*0.22	ME2BUT2ENE + O3= CH3COCH3 + ZCH3CHOOE
6.51E-15*EXP(-829/T)*0.15	ME2BUT2ENE + O3= CH3COCH3 + ECH3CHOOF

Excited CI chemistry	
KDEC*0.35	ZCH3CHOOE = ZCH3CHOO
KDEC*0.65	ZCH3CHOOE = HCOCH2O2 + OH
KDEC*0.35	ECH3CHOOF = ECH3CHOO
KDEC*0.275	ECH3CHOOF = CH4
KDEC*0.167	ECH3CHOOF = CH3OH + CO
KDEC*0.110	ECH3CHOOF = CH2CO
KDEC*0.098	ECH3CHOOF = CH3O2 + HO2
KDEC*0.27	CH3CCH3OOA = CH3CCH3OO
KDEC*0.73	CH3CCH3OOA = CH3COCH2O2 + OH
Stabilized sCI chemistry	
7.2E+06*EXP(-2920/T)	CH3CCH3OO = CH3COCH2O2 + OH
7.54E-18*H2O*0.92	CH3CCH3OO = H2IPROOH
7.54E-18*H2O*0.08	CH3CCH3OO = CH3COCH3 + H2O2
1.82E-14*H2OD*0.87	CH3CCH3OO = H2IPROOH
1.82E-14*H2OD*0.13	CH3CCH3OO = CH3COCH3 + H2O2
3.10E-10	CH3CCH3OO + CH3CO2H = HP2PRACET
1.70E-12	CH3CCH3OO + CH3CHO = IC3SOZC2
3.40E-13	CH3CCH3OO + CH3COCH3 = IC3SOZIC3
3.40E-13	ZCH3CHOO + CH3COCH3 = IC3SOZC2
3.40E-13	ECH3CHOO + CH3COCH3 = IC3SOZC2
OH initiation reactions	
1.92E-11*EXP(450/T)*0.353	ME2BUT2ENE + OH = ME2BU2OLO2
1.92E-11*EXP(450/T)*0.647	ME2BUT2ENE + OH = ME2BUOLO2
RO_2 and RO chemistry	
1.15E-13*EXP(1300/T)*0.18	CH3COCH2O2 + HO2 = CH3COCH2O + OH
1.15E-13*EXP(1300/T)*0.82	CH3COCH2O2 + HO2 = HYPERACET
1.00E-13*EXP(1045/T)*0.2*[RO_2]	CH3COCH2O2 = ACETOL
1.00E-13*EXP(1045/T)*0.6*[RO_2]	CH3COCH2O2 = CH3COCH2O
1.00E-13*EXP(1045/T)*0.2*[RO_2]	CH3COCH2O2 = MGLYOX
KDEC	CH3COCH2O = CH3CO3 + HCHO

4.40E-15*EXP(1910/T)	CH3CO3 + HO2 = CH3CO2H + O3
1.50E-12*EXP(480/T)	CH3CO3 + HO2 = CH3CO3H
4.66E-12*EXP(235/T)	CH3CO3 + HO2 = CH3O2 + OH
2.00E-12*EXP(508/T)*0.2*$[RO_2]$	CH3CO3 = CH3CO2H
2.00E-12*EXP(508/T)*0.8*$[RO_2]$	CH3CO3 = CH3O2
KRO2HO2*0.748	ME2BU2OLO2 + HO2 = M2BU2OLOOH
1.00E-13*EXP(731/T)*0.2*$[RO_2]$	ME2BU2OLO2 = C4ME3HO23
1.00E-13*EXP(731/T)*0.6*$[RO_2]$	ME2BU2OLO2 = ME2BU2OLO
1.00E-13*EXP(731/T)*0.2*$[RO_2]$	ME2BU2OLO2 = MIPKAOH
1.80E+13*EXP(-1424/T)	ME2BU2OLO = CH3COCH3 + CH3CHO + HO2
KRO2HO2*0.748	ME2BUOLO2 + HO2 = ME2BUOLOOH
1.00E-13*EXP(221/T)*0.2*$[RO_2]$	ME2BUOLO2 = C4ME3HO23
1.00E-13*EXP(221/T)*0.8*$[RO_2]$	ME2BUOLO2 = ME2BUOLO
1.80E+13*EXP(-1734/T)	ME2BUOLO = CH3COCH3 + CH3CHO + HO2
2,4,4-Trimethyl-pent-2-ene	
O_3 initiation reactions	
1.42E-16*0.8	TMEPEN2ENE + O3 = TBUTCHO + CH3CCH3OOB
1.42E-16*0.1	TMEPEN2ENE + O3 = CH3COCH3 + ZTBUCHOOA
1.42E-16*0.1	TMEPEN2ENE + O3 = CH3COCH3 + ETBUCHOOA
Excited CI chemistry	
KDEC*0.6	ZTBUCHOOA = ZTBUCHOO
KDEC*0.212	ZTBUCHOOA = IC4H10
KDEC*0.084	ZTBUCHOOA = TBUTOL + CO
KDEC*0.104	ZTBUCHOOA = TC4H9O2 + HO2
KDEC*0.6	ETBUCHOOA = ZTBUCHOO
KDEC*0.212	ETBUCHOOA = IC4H10
KDEC*0.084	ETBUCHOOA = TBUTOL + CO
KDEC*0.104	ETBUCHOOA = TC4H9O2 + HO2
KDEC*0.6	CH3CCH3OOB = CH3CCH3OO
KDEC*0.4	CH3CCH3OOB = CH3COCH2O2 + OH

Stabilized sCI chemistry	
2.58E6*T$^{2.32}$*EXP(-9710/T)	ZTBUCHOO = TBUTCO2H
2.40E-19*H2O*0.73	ZTBUCHOO = TBUCHOHOOH
2.40E-19*H2O*0.06	ZTBUCHOO = TBUTCHO + H2O2
2.40E-19*H2O*0.21	ZTBUCHOO = TBUTCO2H
2.84E-15*H2OD*0.40	ZTBUCHOO = TBUCHOHOOH
2.84E-15*H2OD*0.06	ZTBUCHOO = TBUTCHO + H2O2
2.84E-15*H2OD*0.54	ZTBUCHOO = TBUTCO2H
1.70E-10	ZTBUCHOO + CH3CO2H = HPNPACET
1.70E-12	ZTBUCHOO + CH3CHO = NPC5SOZC2
1.70E-10	ZTBUCHOO + TBUTCO2H = HPNPPIV
1.70E-12	ZTBUCHOO + TBUTCHO = NPSOZNP
3.40E-13	ZTBUCHOO + CH3COCH3 = NPSOZIC3
8.51E9*T$^{1.15}$*EXP(-7357/T)	ETBUCHOO = TBUTCO2H
4.50E-14*H2O*0.73	ETBUCHOO = TBUCHOHOOH
4.50E-14*H2O*0.06	ETBUCHOO = TBUTCHO + H2O2
4.50E-14*H2O*0.21	ETBUCHOO = TBUTCO2H
4.74E-11*H2OD*0.40	ETBUCHOO = TBUCHOHOOH
4.74E-11*H2OD*0.06	ETBUCHOO = TBUTCHO + H2O2
4.74E-11*H2OD*0.54	ETBUCHOO = TBUTCO2H
2.50E-10	ETBUCHOO + CH3CO2H = HPNPACET
1.70E-12	ETBUCHOO + CH3CHO = NPC5SOZC2
2.50E-10	ETBUCHOO + TBUTCO2H = HPNPPIV
1.70E-12	ETBUCHOO + TBUTCHO = NPSOZNP
3.40E-13	ETBUCHOO + CH3COCH3 = NPSOZIC3
3.10E-10	CH3CCH3OO + TBUTCO2H = HP2PRPIV
1.70E-12	CH3CCH3OO + TBUTCHO = NPSOZIC3
OH initiation reactions	
8.0E-11*0.338	TMEPEN2ENE + OH = HOC8AO2
8.0E-11*0.662	TMEPEN2ENE + OH = HOC8BO2
RO$_2$ and RO chemistry	
KRO2HO2*0.601	TC4H9O2 + HO2 = TC4H9OOH

1.00E-13*EXP(-662/T)*0.2*$[RO_2]$	TC4H9O2 = TBUTOL
1.00E-13*EXP(-662/T)*0.8*$[RO_2]$	TC4H9O2 = TC4H9O
6.00E+14*EXP(-8153/T)	TC4H9O = CH3COCH3 + CH3O2
KRO2HO2*0.874	HOC8AO2 + HO2 = HOC8AOOH
1.00E-13*EXP(783/T)*0.2*$[RO_2]$	HOC8AO2 = HOC8ACO
1.00E-13*EXP(783/T)*0.6*$[RO_2]$	HOC8AO2 = HOC8AO
1.00E-13*EXP(783/T)*0.2*$[RO_2]$	HOC8AO2 = HOC8AOH
1.80E+13*EXP(-4076/T)	HOC8AO = CH3COCH3 + TBUTCHO + HO2
KRO2HO2*0.874	HOC8BO2 + HO2 = HOC8BOOH
1.00E-13*EXP(221/T)*0.2*$[RO_2]$	HOC8BO2 = HOC8AOH
1.00E-13*EXP(221/T)*0.8*$[RO_2]$	HOC8BO2 = HOC8BO
1.80E+13*EXP(-1734/T)	HOC8BO = CH3COCH3 + TBUTCHO + HO2
Cyclohexene	
O_3 initiation reactions	
2.80E-15*EXP(-1063/T)*0.62	CHEXENE + O3 = ZC6COCHOOA
2.80E-15*EXP(-1063/T)*0.38	CHEXENE + O3 = EC6COCHOOA
Excited CI chemistry	
KDEC*0.030	ZC6COCHOOA = ZC6COCHOO
KDEC*0.970	ZC6COCHOOA = ADIP2O2 + OH
KDEC*0.030	EC6COCHOOA = EC6COCHOO
KDEC*0.314	EC6COCHOOA = ADIPAL + O
KDEC*0.621	EC6COCHOOA = C4H9CHO
KDEC*0.035	EC6COCHOOA = HCOC4CO2H
Stabilized sCI chemistry	
KDEC	ZC6COCHOO = CHEXSOZ
KDEC	EC6COCHOO = CHEXSOZ
OH initiation reaction	
6.77E-11	CHEXENE + OH = HOCHEXO2
RO_2 and RO chemistry	
KRO2HO2*0.800	HOCHEXO2 + HO2 = HOCHEXOOH

1.00E-13*EXP(760/T)*0.2*$[RO_2]$	HOCHEXO2 = HOCHEXCO
1.00E-13*EXP(760/T)*0.6*$[RO_2]$	HOCHEXO2 = HOCHEXO
1.00E-13*EXP(760/T)*0.2*$[RO_2]$	HOCHEXO2 = HOCHEXOH
KDEC	HOCHEXO = ADIPAL + HO2
2.91E-30*$T^{12.9}$*EXP(-2167/T)	ADIP2O2 = CO6HP5CO3
1.08E-66*$T^{25.23}$*EXP(1616/T)	ADIP2O2 = GLUTAL + CO + OH
5.64E-20*$T^{8.46}$*EXP(945/T)	CO6HP5CO3 = C6HOM1O2
5.64E-20*$T^{8.46}$*EXP(-586/T)	C6HOM1O2 = CO6HP5CO3
2.01E-52*$T^{19.91}$*EXP(1765/T)	CO6HP5CO3 = CO65CO3H + OH
1.08E-66*$T^{25.23}$*EXP(1616/T)	C6HOM1O2 = HCOC3CO3H + CO + OH
KRO2HO2*0.841*0.82	ADIP2O2 + HO2 = ADIP2OOH
KRO2HO2*0.841*0.18	ADIP2O2 + HO2 = ADIP2O + OH
1.00E-13*EXP(878/T)*0.2*$[RO_2]$	ADIP2O2 = ADIP2CO
1.00E-13*EXP(878/T)*0.6*$[RO_2]$	ADIP2O2 = ADIP2O
1.00E-13*EXP(878/T)*0.2*$[RO_2]$	ADIP2O2 = ADIP2OH
KDEC	ADIP2O = GLUTAL + CO + HO2
3.00E-12*EXP(480/T)*0.900	CO6HP5CO3 + HO2 = CO6HP5CO3H
8.83E-15*EXP(1910/T)*0.900	CO6HP5CO3 + HO2 = CO6HP5CO2H + O3
9.35E-12*EXP(235/T)*0.900	CO6HP5CO3 + HO2 = CO5HP4O2 + OH
2.00E-12*EXP(508/T)*0.2*$[RO_2]$	CO6HP5CO3 = CO6HP5CO2H
2.00E-12*EXP(508/T)*0.8*$[RO_2]$	CO6HP5CO3 = CO5HP4O2
KRO2HO2*0.900*0.82	C6HOM1O2 + HO2 = CO6HP5CO3H
KRO2HO2*0.900*0.18	C6HOM1O2 + HO2 = C6HOM1O + OH
1.00E-13*EXP(891/T)*0.2*$[RO_2]$	C6HOM1O2 = CO65CO3H
1.00E-13*EXP(891/T)*0.6*$[RO_2]$	C6HOM1O2 = C6HOM1O
1.00E-13*EXP(891/T)*0.2*$[RO_2]$	C6HOM1O2 = C6HOM1OH
KDEC	C6HOM1O = HCOC3CO3H + CO + HO2
3.48E-25*$T^{10.16}$*EXP(1327/T)	CO5HP4O2 = CO1HP5O2
9.14E-15*$T^{6.76}$*EXP(-423/T)	CO1HP5O2 = CO5HP4O2
2.91E-30*$T^{12.9}$*EXP(-1458/T)	CO5HP4O2 = HP4CHO + CO + OH
1.07E-64*$T^{23.93}$*EXP(3106/T)	CO5HP4O2 = HP5GLYOX + OH

1.08E-66*$T^{25.23}$*EXP(1616/T)	CO1HP5O2 = HP4CHO + CO + OH
KRO2HO2*0.841	CO5HP4O2 + HO2 = CO5HP4OOH
1.00E-13*EXP(821/T)*0.2*[RO_2]	CO5HP4O2 = CO5HP4CHO
1.00E-13*EXP(821/T)*0.6*[RO_2]	CO5HP4O2 = CO5HP4O
1.00E-13*EXP(821/T)*0.2*[RO_2]	CO5HP4O2 = CO5HP4OH
KDEC	CO5HP4O = HOC3H6CHO + CO + OH
KRO2HO2*0.841*0.82	CO1HP5O2 + HO2 = CO5HP4OOH
KRO2HO2*0.841*0.18	CO1HP5O2 + HO2 = CO1HP5O + OH
1.00E-13*EXP(878/T)*0.2*[RO_2]	CO1HP5O2 = HP5GLYOX
1.00E-13*EXP(878/T)*0.6*[RO_2]	CO1HP5O2 = CO1HP5O
1.00E-13*EXP(878/T)*0.2*[RO_2]	CO1HP5O2 = CO1HP5OH
KDEC	CO1HP5O = HP4CHO + CO + HO2
Inorganic reactions	
6.0E-34*[M]*$(T/300)^{-2.6}$*[O_2]	O = O3
8.0E-12*EXP(-2060/T)	O + O3 =
1.70E-12*EXP(-940/T)	OH + O3 = HO2
2.03E-16*$(T/300)^{4.57}$*EXP(693/T)	HO2 + O3 = OH
2.20E-13*EXP(600/T)*F_{H2O} [g]	HO2 + HO2 = H2O2
1.90E-33*[M]*EXP(980/T)*F_{H2O}	HO2 + HO2 = H2O2

Comments

[a] Reaction mechanism is designed for application to single alkene systems, but complete listing must be used for common chemistry to be represented;

[b] Units are cm^3 $molecule^{-1}$ s^{-1} for bimolecular reactions or s^{-1} for unimolecular (or pseudo-unimolecular) reactions;

[c] KDEC is a generic parameter applied to selected very rapid reactions for convenience, and was assigned a value of 1.0E+06 s^{-1} in these calculations;

[d] KMT16 is the rate coefficient for a pressure-dependent reaction in the fall-off regime, with k_0 = 8.0E-27*[M]*$(T/300)^{-3.5}$ cm^3 $molecule^{-1}$ s^{-1}, k_∞ = 3.0E-11*$(T/300)^{-1}$ cm^3 $molecule^{-1}$ s^{-1}, and F_c = 0.5;

[e] KRO2HO2 = 2.80E-13*EXP(1300/T);

[f] [RO_2] represents the concentration sum of all peroxy radicals in the system;

[g] F_{H2O} = 1 + (1.40E-21*EXP(2200/T)*[H_2O]).

245

Table S5: Identities of the organic species in the updated chemical schemes listed in Table S4 [a].

Species	**SMILES** [b]	**Species**	**SMILES**
C3H6	CC=C	C656OH	CCCCC(O)CO
CH2OOA	C=[O+][O-] [c]	C6OH5O	CCCCC([O])CO
CH2OO	C=[O+][O-]	HO5C6O2	CCCCC(O)CO[O]
ZCH3CHOOA	[O-]\[O+]=C/C [c]	HO5C6OOH	CCCCC(O)COO
ZCH3CHOO	[O-]\[O+]=C/C	HO5C5CHO	CCCCC(O)C=O
ECH3CHOOA	[O-]/[O+]=C/C [c]	HO5C6O	CCCCC(O)C[O]
ECH3CHOO	[O-]/[O+]=C/C	HO12C65O2	CC(O[O])CCC(O)CO
HCHO	C=O	HO12C65OOH	CC(OO)CCC(O)CO
CH3CHO	CC=O	HO12C65CO	CC(CCC(O)CO)=O
CH4	C	HO125C6	CC(O)CCC(O)CO
CH3OH	CO	HO12C65O	CC([O])CCC(O)CO
CH2CO	C=C=O	HO15C62CO	CC(O)CCC(CO)=O
HOCH2OOH	OCOO	HO12C64O2	CCC(O[O])CC(O)CO
HCOOH	O=CO	HO12C64OOH	CCC(OO)CC(O)CO
HPMEFORM	O=COCOO	HO12C64CO	CCC(CC(O)CO)=O
HPMEACET	O=C(C)OCOO	HO124C6	CCC(O)CC(O)CO
CSOZC	C1OOCO1	HO12C64O	CCC([O])CC(O)CO
C2SOZC	CC1OOCO1	HO35C5CHO	CCC(O)CC(O)C=O
CH3CHOHOOH	CC(OO)O	CBUT2ENE	C\C=C/C
CH3CO2H	O=C(O)C	ZCH3CHOOB	[O-]\[O+]=C/C [c]
HP1ETFORM	O=COC(C)OO	ECH3CHOOB	[O-]/[O+]=C/C [c]
HP1ETACET	O=C(C)OC(C)OO	BUT2OLO2	[O]OC(C)C(C)O
C2SOZC2	CC1OOC(C)O1	BUT2OLOOH	OOC(C)C(C)O
HCOCH2O2	O=CCO[O]	BUT2OLO	CC(=O)C(C)O
HCOCH2OOH	O=CCOO	BUT2OLOH	CC(O)C(C)O
GLYOX	O=CC=O	BUT2OLAO	CC([O])C(C)O
HOCH2CHO	OCC=O	TBUT2ENE	C/C=C/C
HCOCH2O	[O]CC=O	ECH3CHOOC	[O-]/[O+]=C/C [c]
CH3O2	CO[O]	TPENT2ENE	CC/C=C/C

CH3OOH	COO	ZC2H5CHOOB	[O-]\[O+]=C/CC [c]
CH3O	C[O]	EC2H5CHOOB	[O-]/[O+]=C/CC [c]
HYPROPO2	CC(CO)O[O]	ZCH3CHOOC	[O-]\[O+]=C/C [c]
HYPROPO2H	CC(CO)OO	ECH3CHOOD	[O-]/[O+]=C/C [c]
ACETOL	CC(CO)=O	HP1ETPROP	CCC(OC(C)OO)=O
PROPGLY	CC(CO)O	C3SOZC2	CC1OOC(CC)O1
HYPROPO	CC(CO)[O]	HP1PRACET	CC(OC(CC)OO)=O
IPROPOLO2	CC(CO[O])O	PE2ENEAO2	CCC(O[O])C(O)C
IPROPOLO2H	CC(COO)O	C52OH3OOH	CCC(OO)C(O)C
CH3CHOHCHO	CC(C=O)O	C523OH	CCC(O)C(O)C
IPROPOLO	CC(C[O])O	DIEKAOH	CCC(C(O)C)=O
BUT1ENE	CCC=C	PE2ENEAO	CCC([O])C(O)C
CH2OOB	C=[O+][O-] [c]	PE2ENEBO2	CCC(O)C(O[O])C
ZC2H5CHOOA	[O-]\[O+]=C/CC [c]	C53OH2OOH	CCC(O)C(OO)C
ZC2H5CHOO	[O-]\[O+]=C/CC	MPRKAOH	CCC(O)C(C)=O
EC2H5CHOOA	[O-]/[O+]=C/CC [c]	PE2ENEBO	CCC(O)C([O])C
EC2H5CHOO	[O-]/[O+]=C/CC	THEX2ENE	C/C=C/CCC
C2H6	CC	ZCH3CHOOD	[O-]\[O+]=C/C [c]
C2H5OH	CCO	ECH3CHOOE	[O-]/[O+]=C/C [c]
CH3CHCO	CC=C=O	ZC3H7CHOOB	CCC\C=[O+]/[O-] [c]
PROPACID	CCC(O)=O	EC3H7CHOOB	CCC/C=[O+]/[O-] [c]
C2H5CHO	CCC=O	HP1ETBUTR	O=C(OC(C)OO)CCC
HPMEPROP	O=C(CC)OCOO	C4SOZC2	CC1OOC(CCC)O1
C3SOZC	CCC1OOCO1	HP1BUACET	CC(OC(CCC)OO)=O
ETCHOHOOH	OC(OO)CC	C64OH5O2	CC(O[O])C(O)CCC
HP1PRFORM	O=COC(CC)OO	C64OH5OOH	CC(OO)C(O)CCC
HP1PRPROP	O=C(CC)OC(CC)OO	C645OH	CC(O)C(O)CCC
C3SOZC3	CCC1OOC(CC)O1	CO2HO3C6	CC(C(O)CCC)=O
C2H5O2	CCO[O]	C64OH5O	CC([O])C(O)CCC
C2H5OOH	CCOO	C65OH4O2	CC(O)C(O[O])CCC
C2H5O	CC[O]	C65OH4OOH	CC(O)C(OO)CCC
PROPALO2	CC(O[O])C=O	HEX3ONCOH	CC(O)C(CCC)=O

PROPALOOH	CC(OO)C=O	C65OH4O	CC(O)C([O])CCC
CH3CHOHCHO	CC(O)C=O	ME2BUT2ENE	CC(C)=CC
MGLYOX	CC(C=O)=O	CH3CCH3OOA	CC(C)=[O+][O-] [c]
PROPALO	CC([O])C=O	CH3CCH3OO	CC(C)=[O+][O-]
HO3C4O2	OC(CO[O])CC	ZCH3CHOOE	[O-]\[O+]=C/C [c]
HO3C4OOH	OC(COO)CC	ECH3CHOOF	[O-]\[O+]=C/C [c]
HO3C3CHO	OC(C=O)CC	CH3COCH3	CC(C)=O
NBUTOLAOH	OC(CO)CC	H2IPROOH	CC(C)(OO)O
HO3C4O	OC(C[O])CC	HP2PRACET	CC(C)(OO)OC(C)=O
NBUTOLAO2	CCC(O[O])CO	IC3SOZC2	CC1OOC(C)(C)O1
NBUTOLAOOH	CCC(OO)CO	IC3SOZIC3	CC1(C)OOC(C)(C)O1
MEKCOH	O=C(CO)CC	CH3COCH2O2	CC(CO[O])=O
NBUTOLAO	[O]C(CO)CC	HYPERACET	CC(COO)=O
HO34C4O2	OCC(O)CCO[O]	CH3COCH2O	CC(C[O])=O
HO34C4OOH	OCC(O)CCOO	CH3CO3	CC(O[O])=O
HO34C3CHO	OCC(O)CC=O	CH3CO3H	CC(OO)=O
HO13C4OH	OCC(O)CCO	ME2BU2OLO2	CC(C)(O)C(O[O])C
HO13C3CHO	O=CC(O)CCO	M2BU2OLOOH	CC(C)(O)C(OO)C
HO34C4O	OCC(O)CC[O]	C4ME3HO23	CC(C)(O)C(O)C
PENT1ENE	CCCC=C	MIPKAOH	CC(C)(O)C(C)=O
CH2OOC	C=[O+][O-] [c]	ME2BU2OLO	CC(C)(O)C([O])C
ZC3H7CHOOA	CCC\C=[O+]/[O-] [c]	ME2BUOLO2	CC(C)(O[O])C(O)C
ZC3H7CHOO	CCC\C=[O+]/[O-]	ME2BUOLOOH	CC(C)(OO)C(O)C
EC3H7CHOOA	CCC/C=[O+]/[O-] [c]	ME2BUOLO	CC(C)([O])C(O)C
EC3H7CHOO	CCC/C=[O+]/[O-]	TMEPEN2ENE	CC(C)=CC(C)(C)C
C3H7CHO	CCCC=O	CH3CCH3OOB	CC(C)=[O+][O-] [c]
C3H8	CCC	ZTBUCHOOA	CC(C)(C)/C=[O+]/[O-] [c]
NPROPOL	CCCO	ZTBUCHOO	CC(C)(C)/C=[O+]/[O-]
C2H5CHCO	CCC1=[O]1	ETBUCHOOA	CC(C)(C)/C=[O+]\[O-] [c]
BUTACID	CCCC(O)=O	ETBUCHOO	CC(C)(C)/C=[O+]\[O-]
HPMEBUTR	CCCC(OCOO)=O	IC4H10	CC(C)C
C4SOZC	CCCC1OOCO1	TBUTOL	CC(C)(O)C

PRCHOHOOH	CCCC(OO)O	TBUTCO2H	CC(C)(C(O)=O)C
HP1BUFORM	O=COC(CCC)OO	TBUCHOHOOH	CC(C)(C(O)OO)C
HP1BUBUTR	CCCC(OC(CCC)OO)=O	TBUTCHO	CC(C)(C=O)C
C4SOZC4	CCCC1OOC(CCC)O1	HPNPACET	CC(C)(C(OC(C)=O)OO)C
NC3H7O2	CCCO[O]	NPC5SOZC2	CC1OOC(C(C)(C)C)O1
NC3H7OOH	CCCOO	HPNPPIV	CC(C)(C(OC(C(C)(C)C)=O)OO)C
NC3H7O	CCC[O]	NPSOZNP	CC(C)(C)C1OOC(C(C)(C)C)O1
BUTALAO2	CCC(C=O)O[O]	NPSOZIC3	CC1(C)OOC(C(C)(C)C)O1
BUTALAOOH	CCC(C=O)OO	HP2PRPIV	CC(OC(C(C)(C)C)=O)(C)OO
EGLYOX	CCC(C=O)=O	TC4H9O2	CC(C)(O[O])C
BUTAL2O	CCC(C=O)[O]	TC4H9OOH	CC(C)(OO)C
PE1ENEAO2	CCCC(O[O])CO	TC4H9O	CC(C)([O])C
C51OH2OOH	CCCC(CO)OO	HOC8AO2	CC(C)(O)C(O[O])C(C)(C)C
C51OH2CO	CCCC(=O)CO	HOC8AOOH	CC(C)(O)C(OO)C(C)(C)C
HO12C5	CCCC(O)CO	HOC8ACO	CC(C)(O)C(C(C)(C)C)=O
PE1ENEAO	CCCC([O])CO	HOC8AOH	CC(C)(O)C(O)C(C)(C)C
PE1ENEBO2	CCCC(O)CO[O]	HOC8AO	CC(C)(O)C([O])C(C)(C)C
C52OH1OOH	CCCC(O)COO	HOC8BO2	CC(C)(O[O])C(O)C(C)(C)C
C4OHCHO	CCCC(O)C=O	HOC8BOOH	CC(C)(OO)C(O)C(C)(C)C
PE1ENEBO	CCCC(O)C[O]	HOC8BO	CC(C)([O])C(O)C(C)(C)C
HO12C54O2	OCC(O)CC(C)O[O]	CHEXENE	C1CCCC=C1
HO12C54OOH	OCC(O)CC(C)OO	ZC6COCHOOA	O=CCCCC/C=[O+]\[O-] [c]
C51OH	OCC(O)CC(C)=O	ZC6COCHOO	O=CCCCC/C=[O+]\[O-]
HO124C5	OCC(O)CC(C)O	EC6COCHOOA	O=CCCCC/C=[O+]/[O-] [c]
HO24C4CHO	O=CC(O)CC(C)O	EC6COCHOO	O=CCCCC/C=[O+]/[O-]
HO12C54O	OCC(O)CC(C)[O]	HCOC4CO2H	O=CCCCCC(O)=O
HEX1ENE	CCCCC=C	CHEXSOZ	C12CCCCC(OO2)O1
ZC4H9CHOOA	CCCC\C=[O+]/[O-] [c]	HOCHEXO2	OC1C(O[O])CCCC1
ZC4H9CHOO	CCCC\C=[O+]/[O-]	HOCHEXOOH	OC1C(OO)CCCC1
EC4H9CHOOA	CCCC/C=[O+]/[O-] [c]	HOCHEXCO	OC1C(CCCC1)=O
EC4H9CHOO	CCCC/C=[O+]/[O-]	HOCHEXOH	OC1C(O)CCCC1
C4H9CHO	CCCCC=O	HOCHEXO	OC1C([O])CCCC1

NC4H10	CCCC	ADIPAL	O=CCCCCC=O
NBUTOL	CCCCO	ADIP2O2	O=CCCCC(O[O])C=O
C3H7CHCO	CCCC=C=O	ADIP2OOH	O=CCCCC(OO)C=O
PENTACID	CCCCC(O)=O	ADIP2CO	O=CCCCC(C=O)=O
HPMEPENT	OOCOC(CCCC)=O	ADIP2OH	O=CCCCC(O)C=O
C5SOZC	CCCCC1OOCO1	ADIP2O	O=CCCCC([O])C=O
BUCHOHOOH	OOC(O)CCCC	GLUTAL	O=CCCCC=O
HP1PEFORM	OOC(CCCC)OC=O	CO6HP5CO3	O=C(O[O])CCCC(OO)C=O
HP1PEPENT	OOC(CCCC)OC(CCCC)=O	CO65CO3H	O=C(OO)CCCC(C=O)=O
C5SOZC5	CCCCC1OOC(CCCC)O1	CO6HP5CO3H	O=C(OO)CCCC(OO)C=O
NC4H9O2	CCCCO[O]	CO6HP5CO2H	O=C(O)CCCC(OO)C=O
NC4H9OOH	CCCCOO	C6HOM1O2	O=C(OO)CCCC(O[O])C=O
NC4H9O	CCCC[O]	HCOC3CO3H	O=C(OO)CCCC=O
HO1C4O2	OCCCCO[O]	C6HOM1OH	O=C(OO)CCCC(O)C=O
HO1C4OOH	OCCCCOO	C6HOM1O	O=C(OO)CCCC([O])C=O
HOC3H6CHO	OCCCC=O	CO5HP4O2	O=CC(OO)CCCO[O]
HOC4H8OH	OCCCCO	HP5GLYOX	O=C(C=O)CCCOO
HO1C4O	OCCCC[O]	HP4CHO	O=CCCCOO
C4CHOAO2	CCCC(O[O])C=O	CO5HP4OOH	O=CC(OO)CCCOO
C4CHOAOOH	CCCC(OO)C=O	CO5HP4CHO	O=CCCC(C=O)OO
PGLYOX	CCCC(=O)C=O	CO5HP4OH	OCCCC(C=O)OO
C4CHO2O	CCCC([O])C=O	CO1HP5O2	O=CC(O[O])CCCOO
C6OH5O2	CCCCC(CO)O[O]	CO1HP5OH	OC(C=O)CCCOO
C6OH5OOH	CCCCC(CO)OO	CO1HP5O	[O]C(C=O)CCCOO
C4COMEOH	CCCCC(=O)CO		

Comments

[a] Organic species are listed. Simple inorganic species are represented as follows: Molecular hydrogen (H2), hydroxyl radical (OH), hydroperoxyl radical (HO2), hydrogen peroxide (H2O2), carbon monoxide (CO), ozone (O3) and atomic oxygen (O). Where required, the large excess concentrations of the reagents molecular oxygen, $[O_2]$, water, $[H_2O]$, water dimer, $[(H_2O)_2]$, and bath gas, [M], appear as part of the rate coefficients in Table S4;

[b] Simplified Molecular Input Line Entry System (see: https://www.daylight.com/smiles/index.html);

[c] These are excited Criegee intermediates with varying amounts of excess internal energy, but their SMILES are indistinguishable from the corresponding stabilized Criegee intermediates.

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