Theoretical study of the OH-initiated gas-phase oxidation mechanism of β-pinene ($C_{10}H_{16}$): First generation products

- Supporting Information -

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Naming convention of the intermediates

The intermediates, radicals and closed-shell reaction products, are designated by a base identifier followed by an ordinal, a suffix indicating the type of intermediate, and occasionally modifiers specifying specific conformers of the intermediate. The base identifier is specific to the branch of the mechanism and refers to the initiation site and occasionally also to the sub-branch of the mechanism.

Base identifiers (with ordinal number n) :

Rn : alkyl radical formed following OH-addition on carbon C_a (main addition branch)
ROO6Rn : alkyl radical formed after peroxy radical 6-membered ring closure in **R1OO**
RO5Rn : alkyl radical formed after alkoxy radical 5-membered ring closure in **R1O**
RO6Rn : alkyl radical formed after alkoxy radical 6-membered ring closure in **R1O**
CRn : alkyl radical formed following H-abstraction from carbon C_c
DRn : alkyl radical formed following H-abstraction from carbon C_d
Note that the minor addition branch was not given its own base identifier, as our mechanism did not deviate substantially from the mechanism used in e.g. the MCM; we reused their identifiers.

Suffixes :

(none) : alkyl radical
O : alkoxy radical
OO : alkylperoxy radical
CO : carbonyl product, e.g. as formed in the RO2 + RO2 reactions. Note that this involves removing an additional hydrogen from the base alkyl radical to form the double bond.
OH : hydroxy-substituted product
OOH : hydroperoxide-substituted product.
NO3 : nitrate-substituted product
PAN : peroxyacetylnitrate product

Pm : Generic non-radical product. These products do not necessarily contain the exact alkyl radical substrate suggested by the base identifier used, though obviously the product is closely related to that alkyl radical substrate, and is formed from the substrate in one or a few reaction steps only. An optional "m" can be used to identify different products formed from a common base substrate.

Modifiers :

s, **S** : syn conformer, or derived from a syn-conformer-specific reaction earlier in the mechanism

a, **A** : anti conformer, or derived from an anti-conformer-specific reaction earlier in the mechanism

Exceptions:

Some intermediates in the kinetic model are given names based on either the MCM, on a different semi-systematic naming system, on their systematic or trivial names, or are given an arbitrary name. Examples include:

BPINyl_c, **BPINyl_d** : alkyl radicals formed after H-abstraction on carbons C_c and C_d, respectively.

BPINOH1, **BPINOH2** : alkyl radicals formed after OH-addition on carbons C_a and C_b, respectively.

BPINAO2, **BPINBO2**, **BPINCO2** : MCM names of alkyl peroxy radical intermediates **BPINOH1OO**, **BPINOH2OO**, and **R1OO**, respectively

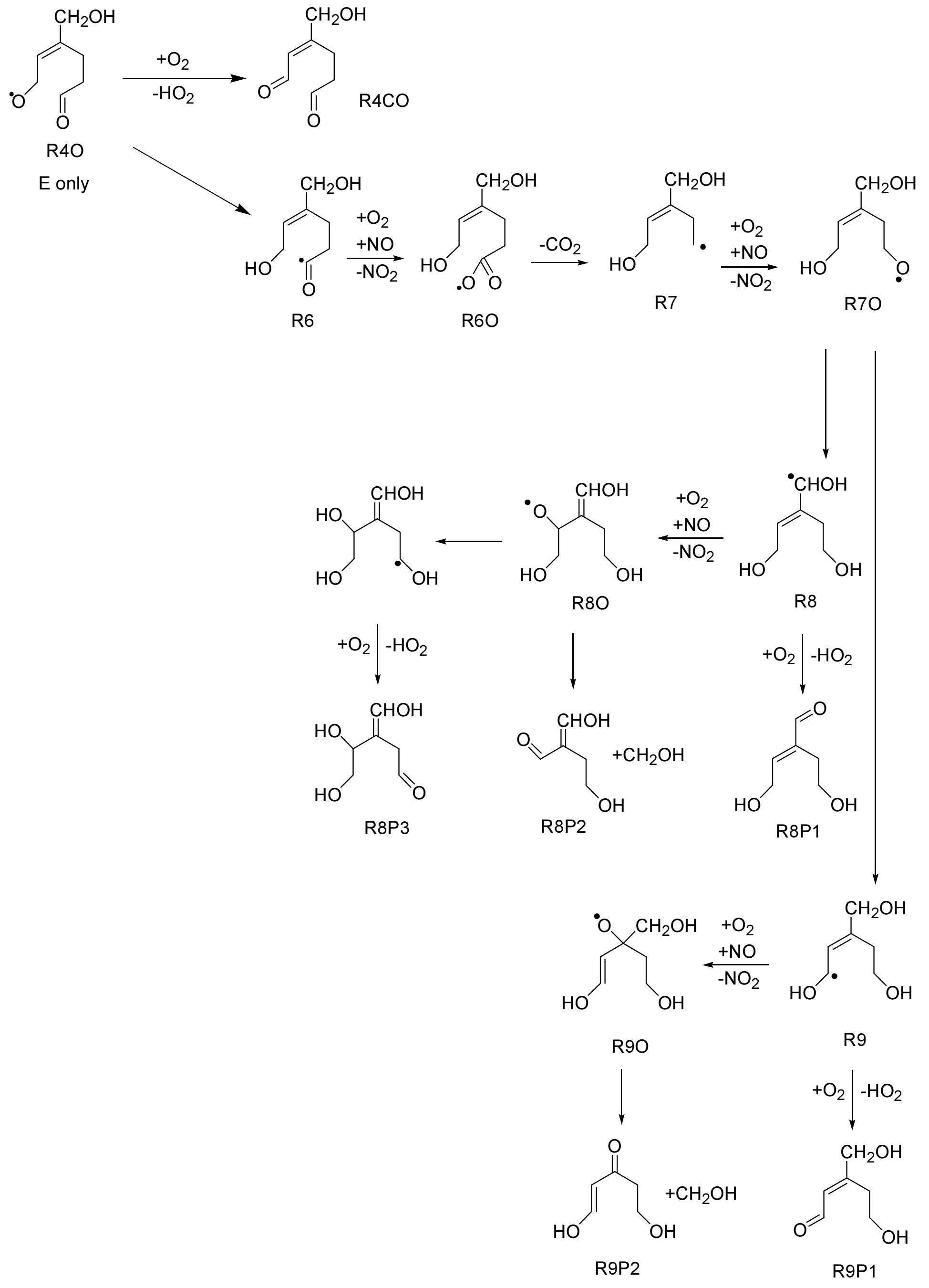
Additional mechanisms

Scheme SI-1: Subsequent fate of R4O

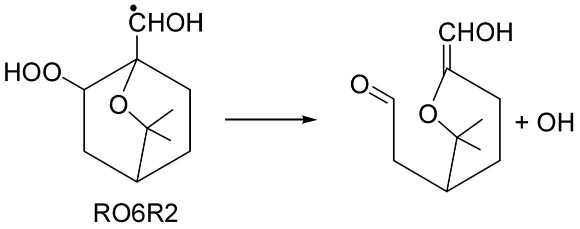
The **R4O** alkoxy radical will, depending on temperature, react with O_2, or undergo a 1,7-H-migration to **R6**; the expected rate for the reaction with O_2 at 1 atm air and 298K is 4.5×10^{4} s^{-1}, while the SAR-predicted rate coefficient for the H-migration is ~4×10^{4} s^{-1} at 298K, accounting for the entropy factor increasing by a factor 1/0.67 due to the presence of a double bond resulting in 1 degree of freedom for internal rotation less in the reactant. The barrier for CH_2O elimination is very high due to the formation of a vinyl radical. The acyl radical **R6** will convert to the acyloxy radical **R6O**, which loses a CO_2 molecule without viable competitive channels, yielding **R7**. The oxy radical subsequently formed, **R7O**, can undergo either a 1,5-H-shift leading to **R8**, or a 1,6-H-shift leading to **R9**. Both of these reaction have comparable rate coefficients, again owing partly to the double bond increasing the entropic factor for the 1,6-H-shift. At 298K, the predicted rate coefficients are 2.4×10^{7} s^{-1} for the 1,5-H-shift, and 2.7×10^{7} s^{-1} for the 1,6-H-shift.

The fate of the **R8** allyl-resonance stabilized radical depends on whether O_2 reacts with the α-hydroxyalkyl moiety, leading to **R8P1** + HO_2, or adds on the alternative radical site, leading in oxidative conditions to the **R8O** alkoxy radical. We propose a 1:1 ratio for these competing O_2 addition channels, lacking unambiguous data to make a better estimate. The **R8O** alkoxy radical can decompose with a SAR-predicted barrier of 5.7 kcal mol^{-1}, leading to **R8P2** + CH_2OH, or less likely undergo another 1,5-H-migration ($k_{isom}(298K) = 2.4\times10^{7}$ s^{-1}) and fast reaction with O_2, leading to **R8P3** + HO_2.

Similar to **R8**, the fate of **R9** depends on which allyl-resonance radical site O_2 reacts with; for reaction in α-position to the hydroxy group, we find **R9P1** + HO_2, for addition on the alternate radical site and conversion to the alkoxy radical **R9O**, we predict formation or **R9P2** + CH_2OH. Again, we propose a ratio of 1:1 for this competition, for lack of more reliable data.


CH2OH
+O2
-HO2
R4O
E only
R4CO
R6
+O2
+NO
-NO2
R6O
-CO2
R7
R7O
HO
O
OH
CHOH
R8O
R8
R8P3
R8P2
+CH2OH
R8P1
R9O
R9
R9P2
R9P1

Scheme SI-2 : ring breaking in RO6R2



The intermediate α-OOH alkyl radical spontaneously decomposes to the aldehyde + OH. The B3LYP barrier height for ring breaking is 22.0 kcal mol^{-1} for the anti conformer and 22.5 kcal mol^{-1} for the syn conformer.

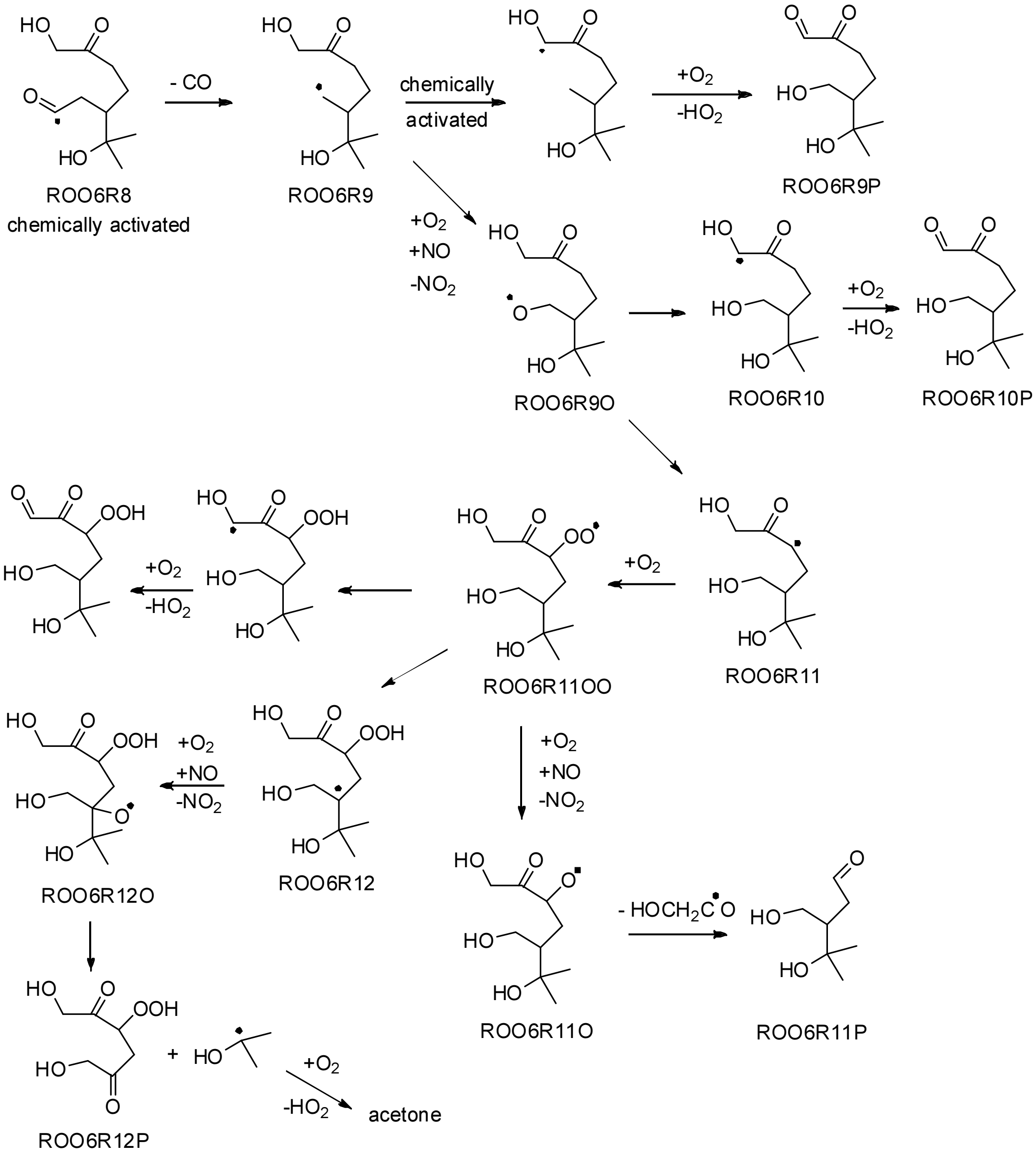
Scheme SI-3 : subsequent chemistry of ROO6R8

The **ROO6R8** radical formed after H-migration in **ROO6R2O** is highly chemically activated, with about 56 kcal mol^{-1} additional internal energy imparted by the **ROO6R1O** alkoxy radical decomposition, the subsequent peroxy radical decomposition, and the 1,5-H-migration. This internal energy is sufficient to promptly eliminate CO, with an energy barrier of the order of 16 kcal mol^{-1}. The fate of the resulting **ROO6R9** radical depends again on the energy still available in this radical; if no energy is lost in collisions throughout the entire formation sequence from **ROO6R1O** the available average energy could still be over 40 kcal mol^{-1}, even when accounting for the 10.9 kcal mol^{-1} endothermic CO elimination step in **ROO6R8**. The required Master Equation and energy redistribution calculations required to determine the energy content of the **ROO6R9** alkyl radical are very demanding, and are omitted at this time as we propose in the main text that the **ROO6R9** radicals are typically not formed.

Chemically activated **ROO6R9** radicals can undergo a 1,6-migration of a hydrogen on the terminal –CH_2OH group; the barrier for this reaction is estimated at 11 kcal mol^{-1} (DFT). Thermalized **ROO6R9** radicals, on the other hand, will preferentially react with O_2, followed by conversion to the **ROO6R9O** alkoxy radical; the intermediate **ROO6R9OO** peroxy radical has no unimolecular reactions that can compete in atmospheric conditions. The **ROO6R9O** alkoxy radical has numerous accessible channels. HCHO elimination, with a SAR barrier of 11.1 kcal mol^{-1}, and 1,5-H-migration of the primary H on the methyl groups, with a B3LYP barrier of 13.54 kcal mol^{-1}, are never competitive. 1,7-H-migration of the α-OH hydrogen (B3LYP barrier of 3.26 kcal mol^{-1}) competes directly against the 1,5-H-migration of the secondary β-oxo hydrogen with a similar barrier of 4.07 kcal mol^{-1} (B3LYP).

The **ROO6R10** α-OH alkyl radical formed after the 1,7-H-migration will react quickly with O_2. The fate of the **ROO6R11OO** peroxy radical generated after the 1,5-H-migration is more complex, with a 1,5-migration of an α-OH secondary H (barrier estimated at 19.58 kcal mol^{-1}), and a 1,5-migration of a tertiary H (barrier estimated at 18.11 kcal mol^{-1}) competing against conversion to the **ROO6R11O** alkoxy radical. Given the barrier heights, it seems unlikely that unimolecular reactions of the **ROO6R11OO** peroxy radical are relevant in atmospheric conditions. For the **ROO6R11O** alkoxy radical, $HOCH_2C^{\bullet}O$ elimination is the lowest barrier decomposition channel (SAR prediction 6.1 kcal mol^{-1}), with the alternative decomposition having a barrier of 12.2 kcal mol^{-1} (SAR). 1,4-H-migration of the α-OH hydrogen is expected to have a high barrier (SAR), while 1,5-H-migration of the other α-OH hydrogen (SAR barrier 5.4 kcal mol^{-1}) has a significant entropic disadvantage compared to decomposition, and is likely to be a minor reaction.

The chemistry shown here is not included in the facsimile kinetic model.

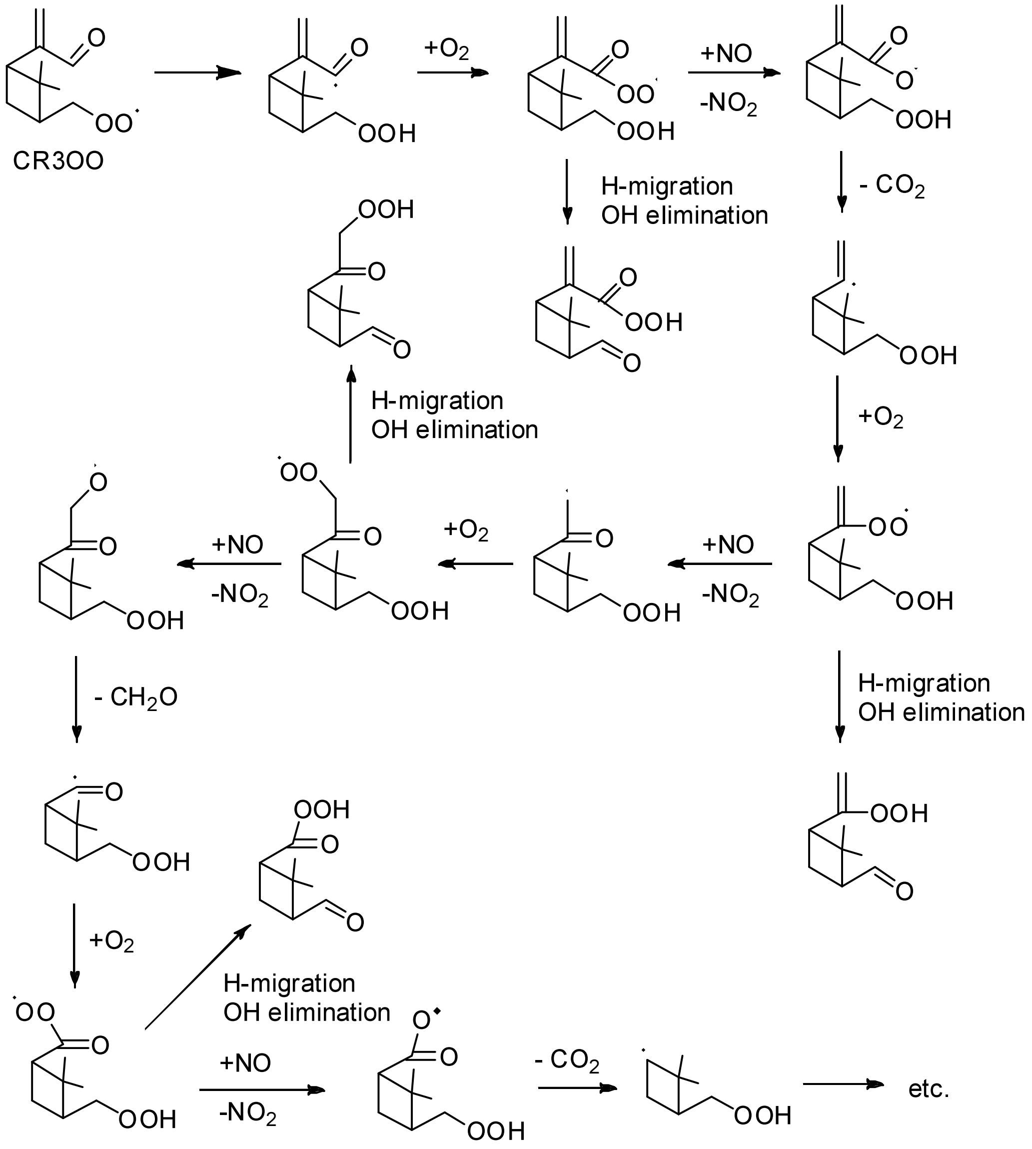


Scheme SI-4 : chemistry of CR3OO after 1,8-H-migration

The scheme below proposes a degradation scheme for the compound formed after H-migration in the C**R3OO** radical. The barrier for 1,8-H-migration in **CR3OO** is predicted by B3LYP to be only 17.5 kcal mol^{-1}; in contrast, calculations on this TS using the CBS-QB3 level of theory yields a barrier of 21.1 kcal mol^{-1}. It is unusual that B3LYP and CBS-QB3 disagree to this extent on the barrier height for this type of reactions; the only other excessive difference was found for the very similar **CR3O** alkoxy radical (see below). Annoyingly, if the B3LYP barrier height is correct, the H-migration can be competitive in pristine conditions, and hence we can not dismiss this chemistry out of hand. Until higher levels of theory can be applied to this specific H-migration, it is undetermined which of the two levels of theory is correct, though CBS-QB3 is nominally the more reliable level of theory.

The main chemistry is fairly standard, and should be well-described using Structure-Activity Relationships; we expect the molecule to break apart into small fragments, including breaking of the 4-membered ring. As the mass flux through this channel is only a small fraction of the β-pinene oxidation, no explicit calculations where performed on this submechanism.

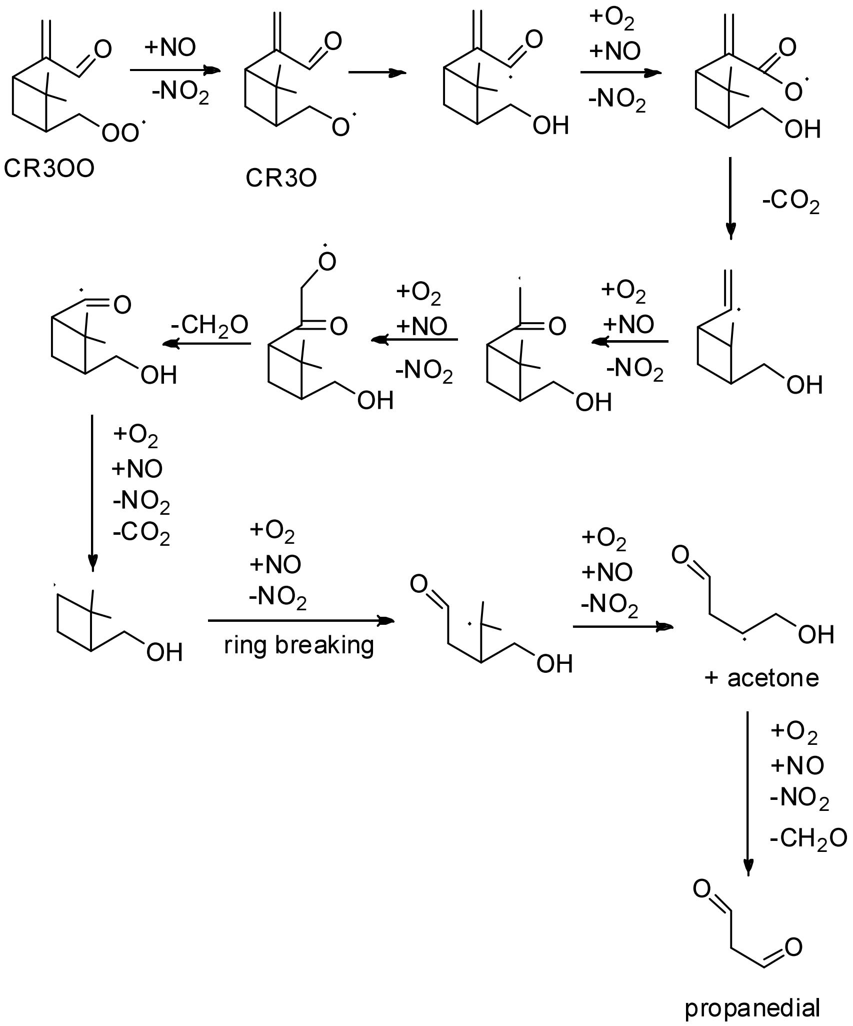
A distinctive feature is the possibility of H-migration of the α-OOH hydrogen, leading to an α-OOH alkyl radical that spontaneously falls apart, regenerating an OH radical. In the mechanism below, it seems this route is accessible for alkylperoxy radicals, with an estimated barrier of 18-20 kcal mol^{-1}. In the alkoxy radical intermediates, the C-C bond scission is expected to outrun H-migrations, though.


CR3OO
+O$_2$
+NO
-NO$_2$
H-migration
OH elimination
- CO$_2$
+O$_2$
H-migration
OH elimination
+NO
-NO$_2$
+O$_2$
+NO
-NO$_2$
H-migration
OH elimination
- CH$_2$O
+O$_2$
H-migration
OH elimination
+NO
-NO$_2$
- CO$_2$
etc.

Scheme SI-5 : chemistry of CR3O after 1,7-H-migration

The scheme below proposes a degradation scheme for the compound formed after H-migration in the C**R3O** radical. The barrier for 1,7-H-migration in **CR3OO** is predicted by B3LYP to be only 7.5 kcal mol^{-1}, in agreement with the H-migration SAR prediction (6.4 kcal mol^{-1}). In contrast, calculations on this TS using the CBS-QB3 level of theory yields a barrier of 11.3 kcal mol^{-1}. This difference is not caused by significant changes in TS geometry between these levels of theory, as single point calculations on the B3LYP geometry (CBS-QB3//B3LYP/6-31G(d,p)) yields a nearly identical barrier height of 12.2 kcal mol^{-1}. Until higher levels of theory can be applied to this specific H-migration, it is undetermined which of the two levels of theory is correct, though CBS-QB3 is considered the more reliable level of theory. If the B3LYP barrier heights are correct, the 1,7-H-migration would likely outrun the 1,5-H-migration, as the barrier height is then lower by a few kcal mol^{-1}, and fewer internal degrees of rotation are lost in the transition state due to the cyclic backbone, the latter counteracting the traditional entropic advantage of migration over a shorter span.

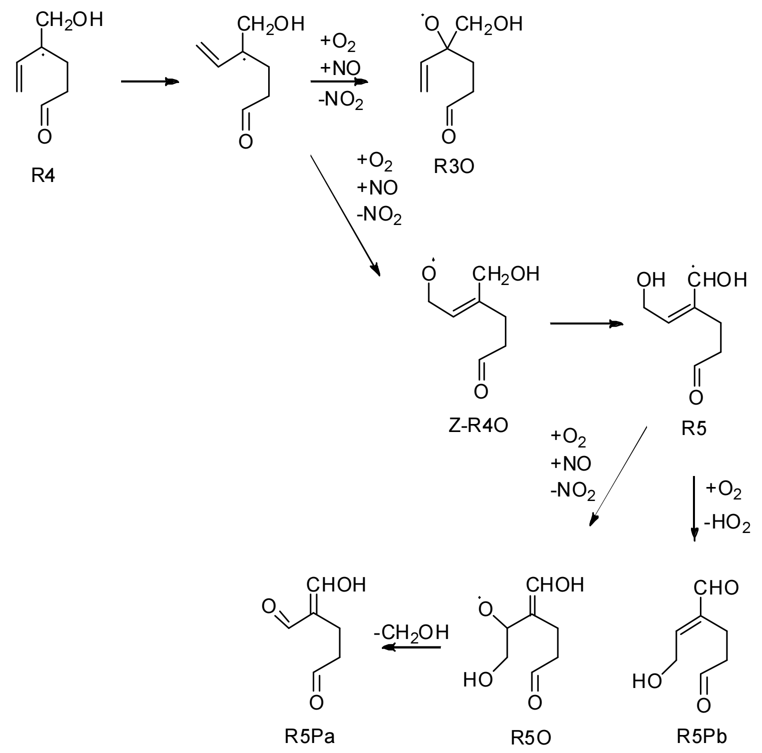
The subsequent chemistry in NO/RO_2/HO_2-rich environment is nearly identical to that of the CR5 radical given in the main text, the main difference being that we expect formation of acetone, rather than hydroxy acetone.


+NO
$-NO_2$
CR3OO
CR3O
$+O_2$
+NO
$-NO_2$
OH
$-CO_2$
$-CH_2O$
ring breaking
+ acetone
propanedial

Additional mechanisms not referenced directly in the main text

Scheme SI-A : chemistry of R4 after internal rotation

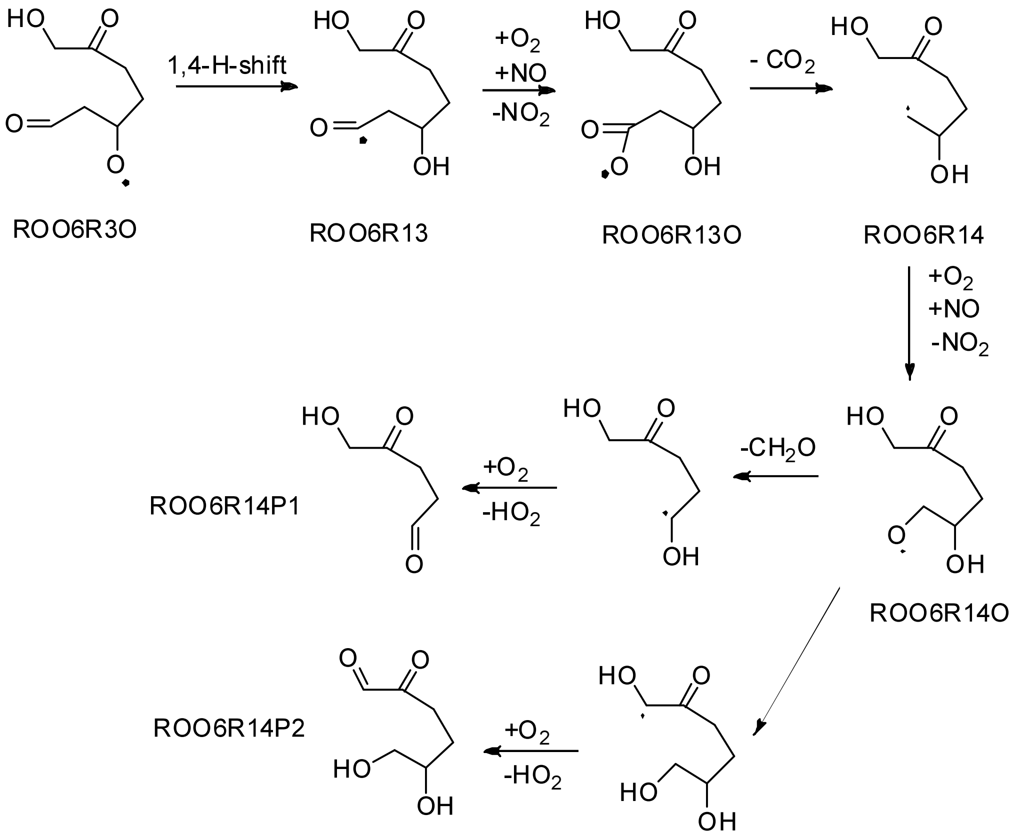
As explained in the main text, it is expected that internal rotation of the partial double bond in alkyl radical **R4** is negligible. For completeness, we do include the chemistry for the Z-conformer of **R4**. Depending on the O_2 addition site in **Z-R4**, one obtains either **R3O** (already discussed in the main text), or **Z-R4O**, after conversion of the alkylperoxy radical to an oxy radical. The facile 1,5-H-shift of the α-OH hydrogen, leaving the **R5** alkyl radical is the fastest accessible unimolecular reaction; this H-shift outruns the 1,7-H-shift and the CH_2O elimination channels. The allyl-resonance-stabilized alkyl radical **R5** can react with O_2 on either of the radical sites. If the O_2 adds on the α-OH radical site, we obtain the hydroxy-dialdehyde **R5Pb**. If the O_2 adds on the secondary alkyl radical site, we obtain an alkoxy radical **R5O** that will quickly eliminate the $^{\bullet}CH_2OH$ radical, leaving a dialdehydic enol.



Scheme SI-B : chemistry of ROO6R3O after 1,4-H-shift

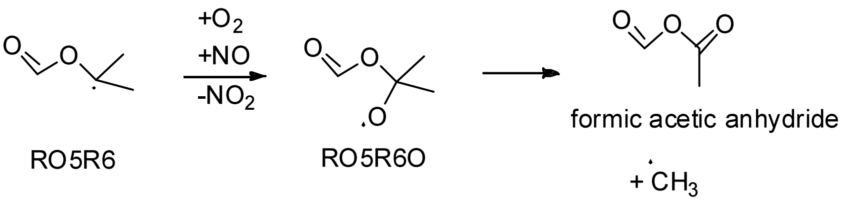
While the barrier for 1,4-migration of the aldehydic hydrogen in **ROO6R3O** was calculated at about 5.5 kcal/mol at the B3LYP level of theory, it was shown that this level of theory can underestimate such barriers significantly; this reaction is then likely negligible. Here, we show the chemistry following the 1,4-H-shift, in case later work shows that this channel should not be neglected.

The acyl radical formed after the 1,4-H-shift, **ROO6R13**, can be converted to an acyloxy radical and eliminate CO_2, leaving a primary radical **ROO6R14**. The alkoxy radical formed from this radical has two accessible channels: HCHO elimination, with a B3LYP barrier of 8.08 kcal mol^{-1}, and the 1,7-H-migration, with a B3LYP barrier of 5.54 kcal mol^{-1}. The relative contribution of these channels will depend on temperature; both reactions form an α-OH alkyl radical that rapidly reacts with O_2, leaving an aldehyde.



Scheme SI-C : chemistry of RO5R6

The peroxy radical **RO5R6OO** is included in the MCM as radical "IPRFORMO2"; however, following the measurements and calculations by Pimentel et al., we prefer to update its chemistry here to form formic acetic anhydride and CH_3 rather than dimethylether, as shown below.



$HC^{\bullet}O$ elimination in **RO5R6** forming acetone directly has a DFT barrier of 23 kcal mol^{-1} and is not competitive.

Kinetic model in Facsimile format

Below, we present a sample implementation of our mechanisms for the OH-initiated oxidation of beta-pinene, for use with the MCM. This implementation uses the MCM protocols for many of the reactions, rather than the SARs listed in the main papers. Hence, it is expected to yield similar, but not identical yields to the mechanism described in the main paper. Furthermore, the kinetic model shown below has not been used in modeling runs, thought earlier versions of it were. As such, it might still contain errors.

Where-ever possible, we used the MCM identifier for the intermediates, to avoid duplicating the chemistry. In a few cases, we update the chemistry in the MCM to such an extend that it is more convenient to use our own identifiers, to avoid conflict with the chemistry currently represented in the MCM. The identifiers following the naming convention of the current paper have an additional "LV" prepended to it to avoid conflict with existing names in the MCM. When merging the partial mechanism below with the MCM, make sure to disable the OH-initiated reactions for beta-pinene already present in the MCM kinetic model, as this will duplicate the chemistry. Some other reactions should be deleted as well, as they are different from our mechanism. These are all indicated with the keyword "DELETE". Some reactions are not included, or not included fully. Products of these reactions are collected in a container "LVSTUFF" to monitor the amount of unspecified products; it should have very minor yields at all times. These reactions are useful mostly for mechanism development, and can be disabled (with or without rescaling of the rate coefficient/branching of the remaining reactions) in a finalized kinetic model.

```
************************************
* List of RO2 species
RO2 = LVCR10OO + LVCR11OO + LVCR1OO + LVCR2OO + LVCR3OO + LVCR4OO +
      LVCR5OO + LVCR6OO + LVCR7OO + LVCR8OO + LVCR9OO + LVCRS1OO +
      LVCRS2OO + LVDR10OO + LVDR11OO + LVDR12OO + LVDR1OO + LVDR2OO +
      LVDR3OO + LVDR4OO + LVDR5OO + LVDR6OO + LVDR7OO + LVDR8OO +
      LVDR9OO + LVR2OO + LVR3OO + LVR4OO + LVR6OO + LVR7OO + LVR8OO +
      LVR9OO + LVRO5R1OO + LVRO5R2OO + LVRO5R3OO + LVRO5R4OO +
      LVRO5R5OO + LVRO5R6OO + LVRO6R3OO + LVROO6R13OO + LVROO6R14OO +
      LVROO6R1OO + LVROO6R3OO + LVROO6R5OO + LVROO6R6OO +
      LVROO6R7OO ;
```

```
**********
**********
**********
* Initiation of the reactions by OH.
*% DELETE : BPINENE + OH = BPINAO2 ;
*% DELETE : BPINENE + OH = BPINBO2 ;
*% DELETE : BPINENE + OH = BPINCO2 ;
* Rate coefficient by Gill and Hites
* Initial branching of BPINENE + OH
% 1.47D-11*EXP(467/TEMP)*0.0681 : BPINENE + OH = BPINBO2 ;
% 1.47D-11*EXP(467/TEMP)*0.8326*0.30 : BPINENE + OH = BPINAO2 ;
% 1.47D-11*EXP(467/TEMP)*0.8326*0.70 : BPINENE + OH = BPINCO2 ;
% 1.47D-11*EXP(467/TEMP)*0.0589 : BPINENE + OH = LVBPINYLc ;
% 1.47D-11*EXP(467/TEMP)*0.0305 : BPINENE + OH = LVBPINYLd ;
* collect minor channels (0.99 % after rounding and summing)
% 1.47D-11*EXP(467/TEMP)*0.0099 : BPINENE + OH = LVSTUFF ;

**********
**********
**********
* Main addition channel
* BPINOH1 (stabilized adduct + O2):
* needs no changes to how it is currently represented in the
* MCM as BPINAO2


**********
* Most reaction of the R1OO radical are already included in the
* MCM as radical BPINCO2, such as the reactions with NO/HO2/RO2
* We add the cyclisation here
% 1.359D9*EXP(-7097/TEMP) : BPINCO2 = LVROO6R1OO ;

**********
* Remove default acetone formation (and incorrect product C720O2)
*% DELETE : BPINCO = C720O2 + CH3COCH3 ;
* cyclisation/dissociation of RO1 oxy radical: 12.4%, 74.1%, 13.5%
% 0.5*KDEC*0.124 : BPINCO = LVRO6R1OOs ;
% 0.5*KDEC*0.124 : BPINCO = LVRO6R1OOa ;
% KDEC*0.741 : BPINCO = LVRO5R1OO ;
% KDEC*0.135 : BPINCO = LVR2OO + CH3COCH3 ;


**********
* reactions of LVRO6R1OO
% KRO2NO*0.747 : LVRO6R1OOs + NO = LVRO6R1O + NO2 ;
% KRO2NO*0.747 : LVRO6R1OOa + NO = LVRO6R1O + NO2 ;
% KRO2NO*0.253 : LVRO6R1OOs + NO = LVRO6R1NO3 ;
% KRO2NO*0.253 : LVRO6R1OOa + NO = LVRO6R1NO3 ;
% KRO2HO2*0.914 : LVRO6R1OOs + HO2 = LVRO6R1OOH ;
% KRO2HO2*0.914 : LVRO6R1OOa + HO2 = LVRO6R1OOH ;
% 0.5*2.17D-12*exp(190/TEMP) : LVRO6R1OOH + OH = LVRO6R1OOs ;
% 0.5*2.17D-12*exp(190/TEMP) : LVRO6R1OOH + OH = LVRO6R1OOs ;
% KRO2NO3 : LVRO6R1OOs + NO3 = LVRO6R1O + NO2 ;
% KRO2NO3 : LVRO6R1OOa + NO3 = LVRO6R1O + NO2 ;
% 8.80D-13*RO2*0.2 : LVRO6R1OOs = LVRO6R1OH ;
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```
% 8.80D-13*RO2*0.2 : LVRO6R1OOs = LVRO6R1CO ;
% 8.80D-13*RO2*0.6 : LVRO6R1OOs = LVRO6R1O ;
% 8.80D-13*RO2*0.2 : LVRO6R1OOa = LVRO6R1OH ;
% 8.80D-13*RO2*0.2 : LVRO6R1OOa = LVRO6R1CO ;
% 8.80D-13*RO2*0.6 : LVRO6R1OOa = LVRO6R1O ;
% 1.43D9*exp(-7851/TEMP) : LVRO6R1OOs = LVRO6R2PP ;
% 1.43D9*exp(-9461/TEMP) : LVRO6R1OOa = LVRO6R2PP ;
* ringbreaking of RO6R1O
% KDEC : LVRO6R1O = LVRO6R3OO ;
% KRO2NO*0.893 : LVRO6R3OO + NO = LVRO6R3O + NO2 ;
% KRO2NO*0.107 : LVRO6R3OO + NO = LVRO6R3NO3 ;
% KRO2HO2*0.914 : LVRO6R3OO + HO2 = LVRO6R3OOH ;
% KRO2NO3 : LVRO6R3OO + NO3 = LVRO6R3O + NO2 ;
% 5.00D-12*RO2*0.3 : LVRO6R3OO = LVRO6R3OH ;
% 5.00D-12*RO2*0.7 : LVRO6R3OO = LVRO6R3O ;
% KDEC : LVRO6R3O = LVRO6R3P ;

**********
* reactions of LVRO5R1OO
% 0.2*KRO2NO*0.894 : LVRO5R1OO + NO = LVRO5R1Os + NO2 ;
% 0.8*KRO2NO*0.894 : LVRO5R1OO + NO = LVRO5R1Oa + NO2 ;
% KRO2NO*0.106 : LVRO5R1OO + NO = LVRO5R1NO3 ;
% KRO2HO2*0.914 : LVRO5R1OO + HO2 = LVRO5R1OOH ;
% 0.2*J<55> : LVRO5R1NO3 = LVRO5R1Os + NO2 ;
% 0.8*J<55> : LVRO5R1NO3 = LVRO5R1Oa + NO2 ;
% 0.2*J<41> : LVRO5R1OOH = LVRO5R1Os + OH ;
% 0.8*J<41> : LVRO5R1OOH = LVRO5R1Oa + OH ;
% 0.5*KRO2NO3 : LVRO5R1OO + NO3 = LVRO5R1Os + NO2 ;
% 0.5*KRO2NO3 : LVRO5R1OO + NO3 = LVRO5R1Oa + NO2 ;
% 9.20D-14*RO2*0.3 : LVRO5R1OO = LVRO5R1OH ;
% 0.5*9.20D-14*RO2*0.7 : LVRO5R1OO = LVRO5R1Os ;
% 0.5*9.20D-14*RO2*0.7 : LVRO5R1OO = LVRO5R1Oa ;
% 1.8E13*exp(-4167/TEMP) : LVRO5R1Os = LVRO5R1P + HCHO + HO2 ;
% 1.8E13*exp(-2869/TEMP) : LVRO5R1Oa = LVRO5R1P + HCHO + HO2 ;
% 1.8E13*exp(-2003/TEMP) : LVRO5R1Os = LVRO5R2OO ;
% 1.8E13*exp(-1902/TEMP) : LVRO5R1Oa = LVRO5R2OO ;
% 0.5*KRO2NO*0.893 : LVRO5R2OO + NO = LVRO5R2Os + NO2 ;
% 0.5*KRO2NO*0.893 : LVRO5R2OO + NO = LVRO5R2Oa + NO2 ;
% KRO2NO*0.107 : LVRO5R2OO + NO = LVRO5R2NO3 ;
% KRO2HO2*0.914 : LVRO5R2OO + HO2 = LVRO5R2OOH ;
% 0.5*KRO2NO3 : LVRO5R2OO + NO3 = LVRO5R2Os + NO2 ;
% 0.5*KRO2NO3 : LVRO5R2OO + NO3 = LVRO5R2Oa + NO2 ;
% 8.80D-13*RO2*0.2 : LVRO5R2OO = LVRO5R2OH ;
% 8.80D-13*RO2*0.2 : LVRO5R2OO = LVRO5R2CO ;
% 0.5*8.80D-13*RO2*0.6 : LVRO5R2OO = LVRO5R2Os ;
% 0.5*8.80D-13*RO2*0.6 : LVRO5R2OO = LVRO5R2Oa ;
% 0.5*J<41> : LVRO5R2OOH = LVRO5R2Os + OH ;
% 0.5*J<41> : LVRO5R2OOH = LVRO5R2Oa + OH ;
% 0.5*J<54> : LVRO5R2NO3 = LVRO5R2Os + NO2  ;
% 0.5*J<54> : LVRO5R2NO3 = LVRO5R2Oa + NO2  ;
* ringbreaking or Hshift in RO5R2O
* judging by CBS-QB3 on Minimum E: Hshift could be 4 kcal/mol higher
% 2.1E10*exp(-2033/TEMP) : LVRO5R2Os = LVRO5R2P ;
% 1.8E13*exp(-2541/TEMP) : LVRO5R2Os = LVRO5R3OO ;
% 1.8E13*exp(-4378/TEMP) : LVRO5R2Oa = LVRO5R3OO ;
% KRO2NO*0.860 : LVRO5R3OO + NO = LVRO5R3O + NO2 ;
% KRO2NO*0.140 : LVRO5R3OO + NO = LVRO5R3NO3 ;
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% KRO2HO2*0.914 : LVRO5R3OO + HO2 = LVRO5R3OOH ;
% KRO2NO3 : LVRO5R3OO + NO3 = LVRO5R3O + NO2 ;
% 1.30D-12*RO2*0.2 : LVRO5R3OO = LVRO56R3OH ;
% 1.30D-12*RO2*0.2 : LVRO5R3OO = LVRO5R3CO ;
% 1.30D-12*RO2*0.6 : LVRO5R3OO = LVRO5R3O ;
* assume only 1,5-H-shift or CH2O elim.
% 8E10*exp(-2859/TEMP) : LVRO5R3O = LVRO5R4OO ;
% 1.8E13*exp(-5445/TEMP) : LVRO5R3O = LVRO5R5OO + HCHO ;
% KRO2NO*0.709 : LVRO5R4OO + NO = LVRO5R4O + NO2 ;
% KRO2NO*0.291 : LVRO5R4OO + NO = LVRO5R4NO3 ;
% KRO2HO2*0.914 : LVRO5R4OO + HO2 = LVRO5R4OOH ;
% KRO2NO3 : LVRO5R4OO + NO3 = LVRO5R4O + NO2 ;
% 8.30D-13*RO2*0.2 : LVRO5R4OO = LVRO5R4OH ;
% 8.30D-13*RO2*0.2 : LVRO5R4OO = LVRO5R4CO ;
% 8.30D-13*RO2*0.6 : LVRO5R4OO = LVRO5R4O ;
% 1.8E13*exp(-2667/TEMP) : LVRO5R4O = LVRO5R4P + CH2OHCOOO ;
% KRO2NO*0.713 : LVRO5R5OO + NO = LVRO5R5O + NO2 ;
% KRO2NO*0.287 : LVRO5R5OO + NO = LVRO5R5NO3 ;
% KRO2HO2*0.890 : LVRO5R5OO + HO2 = LVRO5R5OOH ;
% KRO2NO3 : LVRO5R5OO + NO3 = LVRO5R5O + NO2 ;
% 2.5D-13*RO2*0.2 : LVRO5R5OO = LVRO5R5OH ;
% 2.5D-13*RO2*0.2 : LVRO5R5OO = LVRO5R5CO ;
% 2.5D-13*RO2*0.6 : LVRO5R5OO = LVRO5R5O ;
% 1.8E13*exp(-2818/TEMP) : LVRO5R5O = LVHC5 + LVRO5R6OO ;
% KRO2NO*0.975 : LVRO5R6OO + NO = LVRO5R6O + NO2 ;
% KRO2NO*0.025 : LVRO5R6OO + NO = LVRO5R6NO3 ;
% 1.44D-13 : LVRO5R6NO3 + OH = CH3COCH3 + NO2 ;
% KRO2HO2*0.625 : LVRO5R6OO + HO2 = LVRO5R6OOH ;
% KRO2NO3 : LVRO5R6OO + NO3 = LVRO5R6O + NO2 ;
% 9.2D-14*RO2*0.3 : LVRO5R6OO = LVRO5R6OH ;
% 9.2D-14*RO2*0.7 : LVRO5R6OO = LVRO5R6O ;
% KDEC : LVRO5R6O = FORMACET + CH3O2 ;



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* reactions of LVROO6R1OO
% KRO2NO*0.892 : LVROO6R1OO + NO = LVROO6R1O + NO2 ;
% KRO2NO*0.108 : LVROO6R1OO + NO = LVROO6R1NO3 ;
% KRO2HO2*0.914 : LVROO6R1OO + HO2 = LVROO6R1OOH ;
% KRO2NO3 : LVROO6R1OO + NO3 = LVROO6R1O + NO2 ;
% 1.60D-13*RO2*0.2 : LVROO6R1OO = LVROO6R1OH ;
% 1.60D-13*RO2*0.6 : LVROO6R1OO = LVROO6R1O ;
% 1.60D-13*RO2*0.2 : LVROO6R1OO = LVROO6R1CO ;
% KDEC : LVROO6R1O = LVROO6R2O ;
% KDEC : LVROO6R2O = LVROO6R3OO + CH3COCH3 ;
* not included: 1,5-H-shift of aldehyde-H in LVROO6R2O forming LVROO6R8
% 5.68E10*exp(-8745/TEMP)  : LVROO6R3OO = LVROO6R5OO ;
% KRO2NO*0.890 : LVROO6R3OO + NO = LVROO6R3O + NO2 ;
% KRO2NO*0.010 : LVROO6R3OO + NO = LVROO6R3NO3 ;
% KRO2HO2*0.820 : LVROO6R3OO + HO2 = LVROO6R3OOH ;
% KRO2NO3 : LVROO6R3OO + NO3 = LVROO6R3O + NO2 ;
% 2.50D-13*RO2*0.2 : LVROO6R3OO = LVROO6R3OH ;
% 2.50D-13*RO2*0.6 : LVROO6R3OO = LVROO6R3O ;
% 2.50D-13*RO2*0.2 : LVROO6R3OO = LVROO6R3CO ;
% 5.7E10*exp(-2949/TEMP) : LVROO6R3O = LVROO6R4P + HO2 ;
* Artificially add 2 kcal/mol to the barrier for 1,4-H-shift
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* as B3LYP barrier is likely underestimated. The ROO6R13 branch
* then becomes minor
% 3.6E11*KDEC*exp((-2788-1000)/TEMP) : LVROO6R3O = LVROO6R13OO ;
% KAPNO : LVROO6R13OO + NO = LVROO6R13O + NO2 ;
% KFPAN : LVROO6R13OO + NO2 = LVROO6R13PAN ;
% KBPAN : LVROO6R13PAN = LVROO6R13OO + NO2 ;
% KAPHO2*0.38 : LVROO6R13OO + HO2 = LVROO6R13OOH ;
% KAPHO2*0.12 : LVROO6R13OO + HO2 = LVROO6R13OH + O3 ;
% KAPHO2*0.50 : LVROO6R13OO + HO2 = LVROO6R13O + OH ;
% KRO2NO3 : LVROO6R13OO + NO3 = LVROO6R13O + NO2 ;
% 5.00D-12*RO2*0.3 : LVROO6R13OO = LVROO6R13OH ;
% 5.00D-12*RO2*0.7 : LVROO6R13OO = LVROO6R13O ;
% KDEC : LVROO6R13O = LVROO6R14OO ;
% KRO2NO*0.890 : LVROO6R14OO + NO = LVROO6R14O + NO2 ;
% KRO2NO*0.010 : LVROO6R14OO + NO = LVROO6R14NO3 ;
% KRO2HO2*0.820 : LVROO6R14OO + HO2 = LVROO6R14OOH ;
% KRO2NO3 : LVROO6R14OO + NO3 = LVROO6R14O + NO2 ;
% 2.50D-13*RO2*0.2 : LVROO6R14OO = LVROO6R14OH ;
% 2.50D-13*RO2*0.6 : LVROO6R14OO = LVROO6R14O ;
% 2.50D-13*RO2*0.2 : LVROO6R14OO = LVROO6R14CO ;
% 1.8E13*exp(-4227/TEMP) : LVROO6R14O = HCHO + HO2 + LVROO6R14P ;
* Hshift in peroxy radical, and spontaneous dissociation forming OH
% 9.17E10*exp(-8706/TEMP): LVROO6R5OO = LVROO6R5P + OH ;
% KAPNO : LVROO6R5OO + NO = LVROO6R5O + NO2 ;
% KFPAN : LVROO6R5OO + NO2 = LVROO6R5PAN ;
% KBPAN : LVROO6R5PAN = LVROO6R5OO + NO2 ;
% KAPHO2*0.38 : LVROO6R5OO + HO2 = LVROO6R5OOH ;
% KAPHO2*0.12 : LVROO6R5OO + HO2 = LVROO6R5OH + O3 ;
% KAPHO2*0.50 : LVROO6R5OO + HO2 = LVROO6R5O + OH ;
% KRO2NO3 : LVROO6R5OO + NO3 = LVROO6R5O + NO2 ;
% 5.00D-12*RO2*0.3 : LVROO6R5OO = LVROO6R5OH ;
% 5.00D-12*RO2*0.7 : LVROO6R5OO = LVROO6R5O ;
% KDEC : LVROO6R5O = LVROO6R6OO ;
% KRO2NO*0.871 : LVROO6R6OO + NO = LVROO6R6O + NO2 ;
% KRO2NO*0.129 : LVROO6R6OO + NO = LVROO6R6NO3 ;
% KRO2HO2*0.770 : LVROO6R6OO + HO2 = LVROO6R6OOH ;
% KRO2NO3 : LVROO6R6OO + NO3 = LVROO6R6O + NO2 ;
% 2.00D-12*RO2*0.2 : LVROO6R6OO = LVROO6R6OH ;
% 2.00D-12*RO2*0.6 : LVROO6R6OO = LVROO6R6O ;
% 2.00D-12*RO2*0.2 : LVROO6R6OO = LVROO6R6CO ;
% KDEC : LVROO6R6O = LVROO6R7OO ;
* 1,7-H-peroxyshift
% 8.49E8*exp(-8485/TEMP) : LVROO6R7OO = LVROO6R7P3 + HO2 ;
% KRO2NO*0.722 : LVROO6R7OO + NO = LVROO6R7O + NO2 ;
% KRO2NO*0.278 : LVROO6R7OO + NO = LVROO6R7NO3 ;
% KRO2HO2*0.770 : LVROO6R7OO + HO2 = LVROO6R7OOH ;
% KRO2NO3 : LVROO6R7OO + NO3 = LVROO6R7O + NO2 ;
% 1.40D-12*RO2*0.2 : LVROO6R7OO = LVROO6R7OH ;
% 1.40D-12*RO2*0.6 : LVROO6R7OO = LVROO6R7O ;
% 1.40D-12*RO2*0.2 : LVROO6R7OO = LVROO6R7CO ;
% 5E11*exp(-3298/TEMP) : LVROO6R7O = LVROO6R7P1 + HO2 ;
% 1.8E13*exp(-4227/TEMP) : LVROO6R7O = LVROO6R7P2 + HCHO + HO2 ;


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* reactions of LVR2OO
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% KRO2NO*0.765 : LVR2OO + NO = LVR2O + NO2 ;
% KRO2NO*0.235 : LVR2OO + NO = LVR2NO3 ;
% KRO2HO2*0.820 : LVR2OO + HO2 = LVR2OOH ;
% KRO2NO3 : LVR2OO + NO3 = LVR2O + NO2 ;
% 2.50D-13*RO2*0.2 : LVR2OO = LVR2OH ;
% 2.50D-13*RO2*0.6 : LVR2OO = LVR2O ;
% 2.50D-13*RO2*0.2 : LVR2OO = LVR2CO ;
* Assume 1:1 ratio of primary and tertiary O2 addition on
* allyl-resonance stabilized radical
% KDEC*0.5 : LVR2O = LVR3OO ;
% KDEC*0.5 : LVR2O = LVR4OO ;
% KRO2NO*0.906 : LVR3OO + NO = LVR3O + NO2 ;
% KRO2NO*0.094 : LVR3OO + NO = LVR3NO3 ;
% KRO2HO2*0.820 : LVR3OO + HO2 = LVR3OOH ;
% KRO2NO3 : LVR3OO + NO3 = LVR3O + NO2 ;
% 1.60D-13*RO2*0.3 : LVR3OO = LVR3OH ;
% 1.60D-13*RO2*0.7 : LVR3OO = LVR3O ;
% KDEC : LVR3O = LVR3P + HCHO + HO2 ;
% KRO2NO*0.879 : LVR4OO + NO = LVR4O + NO2 ;
% KRO2NO*0.121 : LVR4OO + NO = LVR4NO3 ;
% KRO2HO2*0.820 : LVR4OO + HO2 = LVR4OOH ;
% KRO2NO3 : LVR4OO + NO3 = LVR4O + NO2 ;
% 2.00D-12*RO2*0.2 : LVR4OO = LVR4OH ;
% 2.00D-12*RO2*0.6 : LVR4OO = LVR4O ;
% 2.00D-12*RO2*0.2 : LVR4OO = LVR4CO ;
* Assume internal rotation around partial double bond in R4 negligible
* This leaves only E-conformers, no Z-conformers
* E-conformer leads to R6; Z-conformer to R5 (disabled)
% KROPRIM*O2 : LVR4O = LVR4CO ;
% 3.0E4/0.726 : LVR4O = LVR6OO ;
*% 2.4E7*0.5 : LVR4O = LVR5Pb + HO2 ;
*% 2.4E7*0.5 : LVR4O = LVR5OO ;
*% KRO2NO*0.730 : LVR5OO + NO = LVR5O + NO2 ;
*% KRO2NO*0.270 : LVR5OO + NO = LVR5NO3 ;
*% KRO2HO2*0.820 : LVR5OO + HO2 = LVR5OOH ;
*% KRO2NO3 : LVR5OO + NO3 = LVR5O + NO2 ;
*% 8.80D-13*RO2*0.2 : LVR5OO = LVR5OH ;
*% 8.80D-13*RO2*0.6 : LVR5OO = LVR5O ;
*% 8.80D-13*RO2*0.2 : LVR5OO = LVR5CO ;
*% KDEC : LVR5O = LVR5Pa + HCHO + HO2 ;
% KAPNO : LVR6OO + NO = LVR6O + NO2 ;
% KFPAN : LVR6OO + NO2 = LVR6PAN ;
% KBPAN : LVR6PAN = LVR6OO + NO2 ;
% KAPHO2*0.38 : LVR6OO + HO2 = LVR6OOH ;
% KAPHO2*0.12 : LVR6OO + HO2 = LVR6OH + O3 ;
% KAPHO2*0.50 : LVR6OO + HO2 = LVR6O + OH ;
% KRO2NO3 : LVR6OO + NO3 = LVR6O + NO2 ;
% 5.00D-12*RO2*0.3 : LVR6OO = LVR6OH ;
% 5.00D-12*RO2*0.7 : LVR6OO = LVR6O ;
% KDEC : LVR6O = LVR7OO ;
% KRO2NO*0.890 : LVR7OO + NO = LVR7O + NO2 ;
% KRO2NO*0.110 : LVR7OO + NO = LVR7NO3 ;
% KRO2HO2*0.770 : LVR7OO + HO2 = LVR7OOH ;
% KRO2NO3 : LVR7OO + NO3 = LVR7O + NO2 ;
% 1.30D-12*RO2*0.2 : LVR7OO = LVR7OH ;
% 1.30D-12*RO2*0.6 : LVR7OO = LVR7O ;
% 1.30D-12*RO2*0.2 : LVR7OO = LVR7CO ;
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% 2.4E7*0.5 : LVR7O = LVR8P1 + HO2 ;
% 2.4E7*0.5 : LVR7O = LVR8OO ;
% (1.8E7/0.67)*0.5 : LVR7O = LVR9P1 + HO2 ;
% (1.8E7/0.67)*0.5 : LVR7O = LVR9OO ;
% KRO2NO*0.743 : LVR8OO + NO = LVR8O + NO2 ;
% KRO2NO*0.257 : LVR8OO + NO = LVR8NO3 ;
% KRO2HO2*0.770 : LVR8OO + HO2 = LVR8OOH ;
% KRO2NO3 : LVR8OO + NO3 = LVR8O + NO2 ;
% 1.40D-12*RO2*0.2 : LVR8OO = LVR8OH ;
% 1.40D-12*RO2*0.2 : LVR8OO = LVR8CO ;
% 1.40D-12*RO2*0.6 : LVR8OO = LVR8O ;
% 1.8e13*exp(-2869/TEMP) : LVR8O = LVR8P2 + HCHO + HO2 ;
% 2.4E7 : LVR8O = LVR8P3 + HO2 ;
% KRO2NO*0.906 : LVR9OO + NO = LVR9O + NO2 ;
% KRO2NO*0.094 : LVR9OO + NO = LVR9NO3 ;
% KRO2HO2*0.770 : LVR9OO + HO2 = LVR9OOH ;
% KRO2NO3 : LVR8OO + NO3 = LVR9O + NO2 ;
% 8.80D-13*RO2*0.2 : LVR9OO = LVR9OH ;
% 8.80D-13*RO2*0.2 : LVR9OO = LVR9CO ;
% 8.80D-13*RO2*0.6 : LVR9OO = LVR9O ;
% KDEC : LVR9O = LVR9P2 + HCHO + HO2 ;

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* Minor addition channel

* Reactions of BPINB and BPINBO2 are in agreement with their current
* representation in the MCM


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* BPINYLC : abstraction of allyl-H

% KDEC*0.5 : LVBPINYLc = LVCR1OO ;
% KDEC*0.5 : LVBPINYLc = LVCR2OO ;

* Reactions of LVCR1OO
% KRO2NO*0.871 : LVCR1OO + NO = LVCR1O + NO2 ;
% KRO2NO*0.129 : LVCR1OO + NO = LVCR1NO3 ;
% KRO2HO2*0.914 : LVCR1OO + HO2 = LVCR1OOH ;
% KRO2NO3 : LVCR1OO + NO3 = LVCR1O + NO2 ;
% 2.00D-12*RO2*0.2 : LVCR1OO = LVCR1OH ;
% 2.00D-12*RO2*0.2 : LVCR1OO = LVCR1CO ;
% 2.00D-12*RO2*0.6 : LVCR1OO = LVCR1O ;
% KROPRIM*O2 : LVCR1O = LVCR1CO + HO2 ;

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* Reactions of LVCR2OO
% KRO2NO*0.730 : LVCR2OO + NO = LVCR2O + NO2 ;
% KRO2NO*0.270 : LVCR2OO + NO = LVCR2NO3 ;
% KRO2HO2*0.914 : LVCR2OO + HO2 = LVCR2OOH ;
% KRO2NO3 : LVCR2OO + NO3 = LVCR2O + NO2 ;
% 1.40D-12*RO2*0.2 : LVCR2OO = LVCR2OH ;
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% 1.40D-12*RO2*0.2 : LVCR2OO = LVCR2CO ;
% 1.40D-12*RO2*0.6 : LVCR2OO = LVCR2O ;
% KDEC*0.5 : LVCR2O = LVCR2Os ;
% KDEC*0.5 : LVCR2O = LVCR2Oa ;
% 1.8E13*exp(-4328/TEMP) : LVCR2Os = LVCRS1OO ;
% 1.8E13*exp(-4730/TEMP) : LVCR2Os = LVCR3OO ;
% KROSEC*O2 : LVCR2Os = LVCR2CO ;
% 1.8E13*exp(-5586/TEMP) : LVCR2Oa = LVCR3OO ;
% KROSEC*O2 : LVCR2Oa = LVCR2CO ;

***********
* reactions of LVCR3OO
* The 1,8-H-shift in LVCR3OO is not included in this mechanism
* as its CBSQB3 barrier of 21.1 kcal/mol makes it negligible
% KRO2NO*0.730 : LVCR3OO + NO = LVCR3O + NO2 ;
% KRO2NO*0.270 : LVCR3OO + NO = LVCR3NO3 ;
% KRO2HO2*0.914 : LVCR3OO + HO2 = LVCR3OOH ;
% KRO2NO3 : LVCR3OO + NO3 = LVCR3O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCR3OO = LVCR3OH ;
% 1.30D-12*RO2*0.2 : LVCR3OO = LVCR3CO ;
% 1.30D-12*RO2*0.6 : LVCR3OO = LVCR3O ;
* The 1,7-H-shift in LVCR3O is not included in this mechanism
* as its CBSQB3 barrier of 11.3 kcal/mol makes its contribution
negligible
% 3.0E4/(0.487) : LVCR3O = LVCR4OO ;
% KROPRIM*O2 : LVCR3O = LVCR3CO ;

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* reactions of LVCR4OO
% 2.3E10*exp(-8857/TEMP) : LVCR4OO = LVCR4OOHP + HO2 ;
% 2.3E10*exp(-8103/TEMP) : LVCR4OO = LVSTUFF ;
% KRO2NO*0.850 : LVCR4OO + NO = LVCR4O + NO2 ;
% KRO2NO*0.150 : LVCR4OO + NO = LVCR4NO3 ;
% KRO2HO2*0.914 : LVCR4OO + HO2 = LVCR4OOH ;
% KRO2NO3 : LVCR4OO + NO3 = LVCR4O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCR4OO = LVCR4OH ;
% 1.30D-12*RO2*0.2 : LVCR4OO = LVCR4CO ;
% 1.30D-12*RO2*0.6 : LVCR4OO = LVCR4O ;
% 3.6E11*exp(-2718/TEMP) : LVCR4OO = LVCR4P + HO2 ;
% 1.43E11*exp(-2466/TEMP) : LVCR4OO = LVCR5OO ;
% 5.72E10*exp(-8556/TEMP) : LVCR5OO = LVCR5P ;
% KAPNO : LVCR5OO + NO = LVCR5O + NO2 ;
% KFPAN : LVCR5OO + NO2 = LVCR5PAN ;
% KBPAN : LVCR5PAN = LVCR5OO + NO2 ;
% KAPHO2*0.38 : LVCR5OO + HO2 = LVCR5OOH ;
% KAPHO2*0.12 : LVCR5OO + HO2 = LVCR5OH + O3 ;
% KAPHO2*0.50 : LVCR5OO + HO2 = LVCR5O + OH ;
% KRO2NO3 : LVCR5OO + NO3 = LVCR5O + NO2 ;
% 1.60D-13*RO2*0.3 : LVCR5OO = LVCR5OH ;
% 1.60D-13*RO2*0.7 : LVCR5OO = LVCR5O ;
% KDEC : LVCR5O = LVCR6OO ;

***********
* reactions of LVCR6OO
% 1.43E11*exp(-8857/TEMP) : LVCR6OO = LVCR6OOHP + HO2 ;
% KRO2NO : LVCR6OO + NO = LVCR6O + NO2 ;
% KRO2HO2*0.914 : LVCR6OO + HO2 = LVCR6OOH ;
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% KRO2NO3 : LVCR6OO + NO3 = LVCR6O + NO2 ;
% 1.30D-12*RO2*0.3 : LVCR6OO = LVCR6OH ;
% 1.30D-12*RO2*0.7 : LVCR6OO = LVCR6O ;
% KDEC : LVCR6O = LVCR7OO ;
% 1.43E11*exp(-8857/TEMP) : LVCR7OO = LVCR7OOHP + HO2 ;
% KRO2NO*0.850 : LVCR7OO + NO = LVCR7O + NO2 ;
% KRO2NO*0.150 : LVCR7OO + NO = LVCR7NO3;
% J<57> : LVCR7NO3 = LVCR8OO + HCHO + NO2 ;
% KRO2HO2*0.914 : LVCR7OO + HO2 = LVCR7OOH ;
% KRO2NO3 : LVCR7OO + NO3 = LVCR7O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCR7OO = LVCR7OH ;
% 1.30D-12*RO2*0.2 : LVCR7OO = LVCR7CO ;
% 1.30D-12*RO2*0.6 : LVCR7OO = LVCR7O ;
% KDEC : LVCR7O = LVCR8OO + HCHO ;
% 1.43E11*exp(-8857/TEMP) : LVCR8OO = LVCR8OOHP + HO2 ;
% KAPNO : LVCR8OO + NO = LVCR8O + NO2 ;
% KFPAN : LVCR8OO + NO2 = LVCR8PAN ;
% KBPAN : LVCR8PAN = LVCR8OO + NO2 ;
% KAPHO2*0.38 : LVCR8OO + HO2 = LVCR8OOH ;
% KAPHO2*0.12 : LVCR8OO + HO2 = LVCR8OH + O3 ;
% KAPHO2*0.50 : LVCR8OO + HO2 = LVCR8O + OH ;
% KRO2NO3 : LVCR8OO + NO3 = LVCR8O + NO2 ;
% 1.60D-13*RO2*0.3 : LVCR8OO = LVCR8OH ;
% 1.60D-13*RO2*0.7 : LVCR8OO = LVCR8O ;
% KDEC : LVCR8O = LVCR9OO ;
% KRO2NO*0.750 : LVCR9OO + NO = LVCR9O + NO2 ;
% KRO2NO*0.250 : LVCR9OO + NO = LVCR9NO3 ;
% KRO2HO2*0.820 : LVCR9OO + HO2 = LVCR9OOH ;
% KRO2NO3 : LVCR9OO + NO3 = LVCR9O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCR9OO = LVCR9OH ;
% 1.30D-12*RO2*0.2 : LVCR9OO = LVCR9CO ;
% 1.30D-12*RO2*0.6 : LVCR9OO = LVCR9O ;
% KDEC : LVCR9O = LVCR10OO + HCHO ;
% 1.43E11*exp(-8857/TEMP) : LVCR10OO = LVCR10OOHP + HO2 ;
% 1.43E11*exp(-8857/TEMP) : LVCR10OO = LVSTUFF + HO2 ;
% KRO2NO*0.900 : LVCR10OO + NO = LVCR10O + NO2 ;
% KRO2NO*0.100 : LVCR10OO + NO = LVCR10NO3 ;
% KRO2HO2*0.820 : LVCR10OO + HO2 = LVCR10OOH ;
% KRO2NO3 : LVCR10OO + NO3 = LVCR10O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCR10OO = LVCR10OH ;
% 1.30D-12*RO2*0.8 : LVCR10OO = LVCR10O ;
% 1.3E7 : LVCR10O = LVSTUFF ;
% 1.9E13*exp(-3271/TEMP) : LVCR10O = LVCR11OO + ACETOL ;
% KRO2NO*0.850 : LVCR11OO + NO = LVCR11O + NO2 ;
% KRO2NO*0.150 : LVCR11OO + NO = LVCR11NO3 ;
% KRO2HO2*0.625 : LVCR11OO + HO2 = LVCR11OOH ;
% KRO2NO3 : LVCR11OO + NO3 = LVCR11O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCR11OO = LVCR11OH ;
% 1.30D-12*RO2*0.2 : LVCR11OO = LVCR11CO ;
% 1.30D-12*RO2*0.6 : LVCR11OO = LVCR11O ;
% KDEC : LVCR11O = HCHO + HCOCH2CHO ;


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* reactions of LVCRS1OO
% KRO2NO*0.867 : LVCRS1OO + NO = LVCRS1O + NO2 ;
% KRO2NO*0.133 : LVCRS1OO + NO = LVCRS1NO3 ;
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% KRO2HO2*0.820 : LVCRS1OO + HO2 = LVCRS1OOH ;
% KRO2NO3 : LVCRS1OO + NO3 = LVCRS1O + NO2 ;
% 1.30D-12*RO2*0.2 : LVCRS1OO = LVCRS1OH ;
% 1.30D-12*RO2*0.2 : LVCRS1OO = LVCRS1CO ;
% 1.30D-12*RO2*0.6 : LVCRS1OO = LVCRS1O ;
% 3E13*exp(-5435/TEMP): LVCRS1O = HCHO + LVSTUFF ;
% 3E13*exp(-4882/TEMP): LVCRS1O = LVCRS2OO ;
* 1,6- alpha-OH peroxy Hshift
% 1.07E12*exp(-8636/TEMP) : LVCRS2OO = LVCRS2OOP ;
% KRO2NO*0.700 : LVCRS2OO + NO = LVCRS2O + NO2 ;
% KRO2NO*0.300 : LVCRS2OO + NO = LVCRS2NO3 ;
% KRO2HO2*0.820 : LVCRS2OO + HO2 = LVCRS2OOH ;
% KRO2NO3 : LVCRS2OO + NO3 = LVCRS2O + NO2 ;
% 1.40D-12*RO2*0.2 : LVCRS2OO = LVCRS2OH ;
% 1.40D-12*RO2*0.2 : LVCRS2OO = LVCRS2CO ;
% 1.40D-12*RO2*0.6 : LVCRS2OO = LVCRS2O ;
% 1.8E13*exp(-2748/TEMP) : LVCRS2O = LVCRS2Pa + HO2 ;
% 2.4E7/0.824 : LVCRS2O = LVCRS2Pb + HO2 ;




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* BPINYLd : strain-enhanced abstraction of hydrogen on Cd

% KDEC : LVBPINYLd = LVDR1OO ;

% KRO2NO*0.72 : LVDR1OO + NO = LVDR1O + NO2 ;
% KRO2NO*0.28 : LVDR1OO + NO = LVDR1NO3 ;
% KRO2HO2*0.914 : LVDR1OO + HO2 = LVDR1OOH ;
% KRO2NO3 : LVDR1OO + NO3 = LVDR1O + NO2 ;
% 2.00D-12*RO2*0.31 : LVDR1OO = LVDR1OH ;
% 2.00D-12*RO2*0.41 : LVDR1OO = LVDR1CO ;
% 2.00D-12*RO2*0.28 : LVDR1OO = LVDR1O ;
* Ring breaking
% KDEC : LVDR1O = LVDR2OO ;

% KRO2NO*0.86 : LVDR2OO + NO = LVDR2O + NO2 ;
% KRO2NO*0.13 : LVDR2OO + NO = LVDR2NO3 ;
% KRO2HO2*0.914 : LVDR2OO + HO2 = LVDR2OOH ;
% KRO2NO3 : LVDR2OO + NO3 = LVDR2O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR2OO = LVDR2OH ;
% 2.00D-12*RO2*0.2 : LVDR2OO = LVDR2CO ;
% 2.00D-12*RO2*0.6 : LVDR2OO = LVDR2O ;
* 1,5-H-shift and 1,6-H-shift
% 8.94D11*exp(-2919/TEMP) : LVDR2O = LVDR3OO ;
% 3.58D11*exp(-3221/TEMP) : LVDR2O = LVDR7OO ;

% KRO2NO*0.72 : LVDR3OO + NO = LVDR3O + NO2 ;
% KRO2NO*0.28 : LVDR3OO + NO = LVDR3NO3 ;
% KRO2HO2*0.914 : LVDR3OO + HO2 = LVDR3OOH ;
% KRO2NO3 : LVDR3OO + NO3 = LVDR3O + NO2 ;
% 2.00D-12*RO2*0.32 : LVDR3OO = LVDR3OH ;
% 2.00D-12*RO2*0.41 : LVDR3OO = LVDR3CO ;
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% 2.00D-12*RO2*0.27 : LVDR3OO = LVDR3O ;
% 1.8D13*exp(-151/TEMP)*0.5 : LVDR3O = LVDR4OO ;
% 1.8D13*exp(-151/TEMP)*0.5 : LVDR3O = LVDR6OO ;
% 1.8D13*exp(-654/TEMP) : LVDR3O = LVDR5OO ;

% KRO2NO*0.72 : LVDR4OO + NO = LVDR4O + NO2 ;
% KRO2NO*0.28 : LVDR4OO + NO = LVDR4NO3 ;
% KRO2HO2*0.914 : LVDR4OO + HO2 = LVDR4OOH ;
% KRO2NO3 : LVDR4OO + NO3 = LVDR4O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR4OO = LVDR4OH ;
% 2.00D-12*RO2*0.2 : LVDR4OO = LVDR4CO ;
% 2.00D-12*RO2*0.6 : LVDR4OO = LVDR4O ;
* 1,5-H-migration vrs decomposition
% 2.86D11*exp(-2013/TEMP) : LVDR4O = LVSTUFF ;
% 1.8D13*exp(-1862/TEMP) : LVDR4O = LVDR10OO + HMACR ;
% KRO2NO*0.72 : LVDR10OO + NO = LVDR10O + NO2 ;
% KRO2NO*0.28 : LVDR10OO + NO = LVDR10NO3 ;
% KRO2HO2*0.914 : LVDR10OO + HO2 = LVDR10OOH ;
% KRO2NO3 : LVDR10OO + NO3 = LVDR10O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR10OO = LVDR10OH ;
% 2.00D-12*RO2*0.8 : LVDR10OO = LVDR10O ;
% KDEC : LVDR10O = C3DIALOO + CH3COCH3 ;

% KRO2NO*0.85 : LVDR6OO + NO = LVDR6O + NO2 ;
% KRO2NO*0.15 : LVDR6OO + NO = LVDR6NO3 ;
% KRO2HO2*0.914 : LVDR6OO + HO2 = LVDR6OOH ;
% KRO2NO3 : LVDR6OO + NO3 = LVDR6O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR6OO = LVDR6OH ;
% 2.00D-12*RO2*0.2 : LVDR6OO = LVDR6CO ;
% 2.00D-12*RO2*0.6 : LVDR6OO = LVDR6O ;
% KDEC : LVDR6O = LVSTUFF ;

% KRO2NO*0.72 : LVDR5OO + NO = LVDR5O + NO2 ;
% KRO2NO*0.28 : LVDR5OO + NO = LVDR5NO3 ;
% KRO2HO2*0.914 : LVDR5OO + HO2 = LVDR5OOH ;
% KRO2NO3 : LVDR5OO + NO3 = LVDR5O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR5OO = LVDR5OH ;
% 2.00D-12*RO2*0.2 : LVDR5OO = LVDR5CO ;
% 2.00D-12*RO2*0.6 : LVDR5OO = LVDR5O ;
% KDEC : LVDR5O = LVDR11OO + GLYOX ;

% KRO2NO*0.90 : LVDR11OO + NO = LVDR11O + NO2 ;
% KRO2NO*0.10 : LVDR11OO + NO = LVDR11NO3 ;
% KRO2HO2*0.770 : LVDR11OO + HO2 = LVDR11OOH ;
% KRO2NO3 : LVDR11OO + NO3 = LVDR11O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR11OO = LVDR11OH ;
% 2.00D-12*RO2*0.8 : LVDR11OO = LVDR11O ;
% KDEC : LVDR11O = LVDR12OO + CH3COCH3 ;
% KDEC : LVDR12OO = LVSTUFF ;


% KAPNO : LVDR7OO + NO = LVDR7O + NO2 ;
% KFPAN : LVDR7OO + NO2 = LVDR7OOPAN ;
% KBPAN : LVDR7OOPAN = LVDR7OO + NO2 ;
% KAPHO2*0.38 : LVDR7OO + HO2 = LVDR7OOH ;
% KAPHO2*0.12 : LVDR7OO + HO2 = LVDR7OH + O3 ;
% KAPHO2*0.50 : LVDR7OO + HO2 = LVDR7O + OH ;
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% KRO2NO3 : LVDR7OO + NO3 = LVDR7O + NO2 ;
% 5.00D-12*RO2*0.3 : LVDR7OO = LVDR7OH ;
% 5.00D-12*RO2*0.7 : LVDR7OO = LVDR7O ;
* CO2 elimination
% KDEC : LVDR7O = LVDR8OO ;

% KRO2NO*0.72 : LVDR8OO + NO = LVDR8O + NO2 ;
% KRO2NO*0.28 : LVDR8OO + NO = LVDR8NO3 ;
% KRO2HO2*0.890 : LVDR8OO + HO2 = LVDR8OOH ;
% KRO2NO3 : LVDR8OO + NO3 = LVDR8O + NO2 ;
% 2.00D-12*RO2*0.32 : LVDR8OO = LVDR8OH ;
% 2.00D-12*RO2*0.41 : LVDR8OO = LVDR8CO ;
% 2.00D-12*RO2*0.27 : LVDR8OO = LVDR8O ;
* peroxy 1,7-H-shift
% 4.6D10*exp(-5536/TEMP) : LVDR800 = LVDR8P ;
* alkoxy radical 2 ring openings
% 1.8D13*exp(-1308/TEMP) : LVDR8O = LVSTUFF ;
% 1.8D13*exp(-302/TEMP) : LVDR8O = LVDR9OO ;

% KRO2NO*0.89 : LVDR9OO + NO = LVDR9O + NO2 ;
% KRO2NO*0.11 : LVDR9OO + NO = LVDR9NO3 ;
% KRO2HO2*0.914 : LVDR9OO + HO2 = LVDR9OOH ;
% KRO2NO3 : LVDR9OO + NO3 = LVDR9O + NO2 ;
% 2.00D-12*RO2*0.2 : LVDR9OO = LVDR9OH ;
% 2.00D-12*RO2*0.8 : LVDR9OO = LVDR9O ;
% KDEC : LVDR9O = LVSTUFF + CH3COCH3 ;




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* AUTOGENERATED reactions
*   - photolysis of hydroperoxides
*   - H-abstraction from hydroperoxides
*   - alpha-H-abstraction from hydroperoxides
*   - photolysis of nitrates
*   - H-abstraction from nitrates
*   - Dilution of all species
% J<41> : LVR4OOH = LVR4O + OH ;
% 1.90D-12*exp(190/TEMP) : LVR4OOH + OH = LVR4OO ;
% 1.10D-11 : LVR4OOH + OH = LVR4CO + OH ;
% J<41> : LVDR7OOH = LVDR7O + OH ;
% 4.42D-12 : LVDR7OOH + OH = LVDR7OO ;
% J<41> : LVRO6R3OOH = LVRO6R3O + OH ;
% 2.17D-12*exp(190/TEMP) : LVRO6R3OOH + OH = LVRO6R3OO ;
% J<41> : LVCR11OOH = LVCR11O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR11OOH + OH = LVCR11OO ;
% 1.66D-11 : LVCR11OOH + OH = LVCR11CO + OH ;
% J<41> : LVROO6R3OOH = LVROO6R3O + OH ;
% 1.90D-12*exp(190/TEMP) : LVROO6R3OOH + OH = LVROO6R3OO ;
% 1.66D-11 : LVROO6R3OOH + OH = LVROO6R3CO + OH ;
% J<41> : LVRO6R1OOH = LVRO6R1O + OH ;
% 1.66D-11 : LVRO6R1OOH + OH = LVRO6R1CO + OH ;
% J<41> : LVDR1OOH = LVDR1O + OH ;
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% 1.90D-12*exp(190/TEMP) : LVDR1OOH + OH = LVDR1OO ;
% 1.66D-11 : LVDR1OOH + OH = LVDR1CO + OH ;
% J<41> : LVCR3OOH = LVCR3O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR3OOH + OH = LVCR3OO ;
% 1.10D-11 : LVCR3OOH + OH = LVCR3CO + OH ;
% J<41> : LVDR4OOH = LVDR4O + OH ;
% 1.90D-12*exp(190/TEMP) : LVDR4OOH + OH = LVDR4OO ;
% 1.66D-11 : LVDR4OOH + OH = LVDR4CO + OH ;
% J<41> : LVROO6R14OOH = LVROO6R14O + OH ;
% 1.90D-12*exp(190/TEMP) : LVROO6R14OOH + OH = LVROO6R14OO ;
% 1.10D-11 : LVROO6R14OOH + OH = LVROO6R14CO + OH ;
% J<41> : LVDR6OOH = LVDR6O + OH ;
% 1.90D-12*exp(190/TEMP) : LVDR6OOH + OH = LVDR6OO ;
% 1.10D-11 : LVDR6OOH + OH = LVDR6CO + OH ;
% 2.17D-12*exp(190/TEMP) : LVRO5R1OOH + OH = LVRO5R1OO ;
% J<41> : LVROO6R1OOH = LVROO6R1O + OH ;
% 2.17D-12*exp(190/TEMP) : LVROO6R1OOH + OH = LVROO6R1OO ;
% J<41> : LVCR1OOH = LVCR1O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR1OOH + OH = LVCR1OO ;
% 1.10D-11 : LVCR1OOH + OH = LVCR1CO + OH ;
% J<41> : LVRO5R3OOH = LVRO5R3O + OH ;
% 1.90D-12*exp(190/TEMP) : LVRO5R3OOH + OH = LVRO5R3OO ;
% 1.10D-11 : LVRO5R3OOH + OH = LVRO5R3CO + OH ;
% J<41> : LVROO6R5OOH = LVROO6R5O + OH ;
% 4.42D-12 : LVROO6R5OOH + OH = LVROO6R5OO ;
% J<41> : LVR9OOH = LVR9O + OH ;
% 1.90D-12*exp(190/TEMP) : LVR9OOH + OH = LVR9OO ;
% 1.66D-11 : LVR9OOH + OH = LVR9CO + OH ;
% J<41> : LVDR8OOH = LVDR8O + OH ;
% 1.90D-12*exp(190/TEMP) : LVDR8OOH + OH = LVDR8OO ;
% 1.66D-11 : LVDR8OOH + OH = LVDR8CO + OH ;
% J<41> : LVDR11OOH = LVDR11O + OH ;
% 2.17D-12*exp(190/TEMP) : LVDR11OOH + OH = LVDR11OO ;
% J<41> : LVDR3OOH = LVDR3O + OH ;
% 1.90D-12*exp(190/TEMP) : LVDR3OOH + OH = LVDR3OO ;
% 1.66D-11 : LVDR3OOH + OH = LVDR3CO + OH ;
% J<41> : LVCR2OOH = LVCR2O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR2OOH + OH = LVCR2OO ;
% 1.66D-11 : LVCR2OOH + OH = LVCR2CO + OH ;
% J<41> : LVROO6R7OOH = LVROO6R7O + OH ;
% 1.90D-12*exp(190/TEMP) : LVROO6R7OOH + OH = LVROO6R7OO ;
% 1.66D-11 : LVROO6R7OOH + OH = LVROO6R7CO + OH ;
% J<41> : LVCR7OOH = LVCR7O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR7OOH + OH = LVCR7OO ;
% 1.10D-11 : LVCR7OOH + OH = LVCR7CO + OH ;
% J<41> : LVCR8OOH = LVCR8O + OH ;
% 4.42D-12 : LVCR8OOH + OH = LVCR8OO ;
% J<41> : LVDR10OOH = LVDR10O + OH ;
% 2.17D-12*exp(190/TEMP) : LVDR10OOH + OH = LVDR10OO ;
% J<41> : LVR2OOH = LVR2O + OH ;
% 1.90D-12*exp(190/TEMP) : LVR2OOH + OH = LVR2OO ;
% 1.66D-11 : LVR2OOH + OH = LVR2CO + OH ;
% J<41> : LVDR5OOH = LVDR5O + OH ;
% 1.90D-12*exp(190/TEMP) : LVDR5OOH + OH = LVDR5OO ;
% 1.66D-11 : LVDR5OOH + OH = LVDR5CO + OH ;
% J<41> : LVR7OOH = LVR7O + OH ;
% 1.90D-12*exp(190/TEMP) : LVR7OOH + OH = LVR7OO ;
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% 1.10D-11 : LVR7OOH + OH = LVR7CO + OH ;
% J<41> : LVCRS2OOH = LVCRS2O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCRS2OOH + OH = LVCRS2OO ;
% 1.66D-11 : LVCRS2OOH + OH = LVCRS2CO + OH ;
% J<41> : LVCR10OOH = LVCR10O + OH ;
% 2.17D-12*exp(190/TEMP) : LVCR10OOH + OH = LVCR10OO ;
% J<41> : LVRO5R4OOH = LVRO5R4O + OH ;
% 1.90D-12*exp(190/TEMP) : LVRO5R4OOH + OH = LVRO5R4OO ;
% 1.66D-11 : LVRO5R4OOH + OH = LVRO5R4CO + OH ;
% J<41> : LVR6OOH = LVR6O + OH ;
% 4.42D-12 : LVR6OOH + OH = LVR6OO ;
% J<41> : LVCR9OOH = LVCR9O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR9OOH + OH = LVCR9OO ;
% 1.66D-11 : LVCR9OOH + OH = LVCR9CO + OH ;
% J<41> : LVROO6R6OOH = LVROO6R6O + OH ;
% 1.90D-12*exp(190/TEMP) : LVROO6R6OOH + OH = LVROO6R6OO ;
% 1.10D-11 : LVROO6R6OOH + OH = LVROO6R6CO + OH ;
% J<41> : LVCRS1OOH = LVCRS1O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCRS1OOH + OH = LVCRS1OO ;
% 1.10D-11 : LVCRS1OOH + OH = LVCRS1CO + OH ;
% J<41> : LVCR6OOH = LVCR6O + OH ;
% 2.17D-12*exp(190/TEMP) : LVCR6OOH + OH = LVCR6OO ;
% J<41> : LVRO5R6OOH = LVRO5R6O + OH ;
% 2.17D-12*exp(190/TEMP) : LVRO5R6OOH + OH = LVRO5R6OO ;
% J<41> : LVDR2OOH = LVDR2O + OH ;
% 1.90D-12*exp(190/TEMP) : LVDR2OOH + OH = LVDR2OO ;
% 1.10D-11 : LVDR2OOH + OH = LVDR2CO + OH ;
% J<41> : LVR3OOH = LVR3O + OH ;
% 2.17D-12*exp(190/TEMP) : LVR3OOH + OH = LVR3OO ;
% J<41> : LVCR5OOH = LVCR5O + OH ;
% 4.42D-12 : LVCR5OOH + OH = LVCR5OO ;
% J<41> : LVRO5R5OOH = LVRO5R5O + OH ;
% 1.90D-12*exp(190/TEMP) : LVRO5R5OOH + OH = LVRO5R5OO ;
% 1.66D-11 : LVRO5R5OOH + OH = LVRO5R5CO + OH ;
% J<41> : LVDR9OOH = LVDR9O + OH ;
% 2.17D-12*exp(190/TEMP) : LVDR9OOH + OH = LVDR9OO ;
% J<41> : LVROO6R13OOH = LVROO6R13O + OH ;
% 4.42D-12 : LVROO6R13OOH + OH = LVROO6R13OO ;
% 1.90D-12*exp(190/TEMP) : LVRO5R2OOH + OH = LVRO5R2OO ;
% 1.66D-11 : LVRO5R2OOH + OH = LVRO5R2CO + OH ;
% J<41> : LVR8OOH = LVR8O + OH ;
% 1.90D-12*exp(190/TEMP) : LVR8OOH + OH = LVR8OO ;
% 1.66D-11 : LVR8OOH + OH = LVR8CO + OH ;
% J<41> : LVCR4OOH = LVCR4O + OH ;
% 1.90D-12*exp(190/TEMP) : LVCR4OOH + OH = LVCR4OO ;
% 1.10D-11 : LVCR4OOH + OH = LVCR4CO + OH ;
% J<53> : LVDR2NO3 = LVDR2O + NO2  ;
% 7.30D-13 : LVDR2NO3 + OH = LVDR2CO + NO2  ;
% J<54> : LVDR1NO3 = LVDR1O + NO2  ;
% 9.16D-13 : LVDR1NO3 + OH = LVDR1CO + NO2  ;
% J<54> : LVDR5NO3 = LVDR5O + NO2  ;
% 9.16D-13 : LVDR5NO3 + OH = LVDR5CO + NO2  ;
% J<55> : LVCR10NO3 = LVCR10O + NO2  ;
% J<54> : LVDR4NO3 = LVDR4O + NO2  ;
% 9.16D-13 : LVDR4NO3 + OH = LVDR4CO + NO2  ;
% J<54> : LVCR11NO3 = LVCR11O + NO2  ;
% 9.16D-13 : LVCR11NO3 + OH = LVCR11CO + NO2  ;
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% J<55> : LVDR11NO3 = LVDR11O + NO2  ;
% J<53> : LVCRS1NO3 = LVCRS1O + NO2  ;
% 7.30D-13 : LVCRS1NO3 + OH = LVCRS1CO + NO2  ;
% J<53> : LVCR1NO3 = LVCR1O + NO2  ;
% 7.30D-13 : LVCR1NO3 + OH = LVCR1CO + NO2  ;
% J<54> : LVCRS2NO3 = LVCRS2O + NO2  ;
% 9.16D-13 : LVCRS2NO3 + OH = LVCRS2CO + NO2  ;
% J<53> : LVRO5R3NO3 = LVRO5R3O + NO2  ;
% 7.30D-13 : LVRO5R3NO3 + OH = LVRO5R3CO + NO2  ;
% J<54> : LVRO5R5NO3 = LVRO5R5O + NO2  ;
% 9.16D-13 : LVRO5R5NO3 + OH = LVRO5R5CO + NO2  ;
% J<53> : LVCR4NO3 = LVCR4O + NO2  ;
% 7.30D-13 : LVCR4NO3 + OH = LVCR4CO + NO2  ;
% J<53> : LVR4NO3 = LVR4O + NO2  ;
% 7.30D-13 : LVR4NO3 + OH = LVR4CO + NO2  ;
% J<55> : LVR3NO3 = LVR3O + NO2  ;
% J<53> : LVCR3NO3 = LVCR3O + NO2  ;
% 7.30D-13 : LVCR3NO3 + OH = LVCR3CO + NO2  ;
% J<53> : LVR7NO3 = LVR7O + NO2  ;
% 7.30D-13 : LVR7NO3 + OH = LVR7CO + NO2  ;
% J<55> : LVRO5R6NO3 = LVRO5R6O + NO2  ;
% J<54> : LVCR2NO3 = LVCR2O + NO2  ;
% 9.16D-13 : LVCR2NO3 + OH = LVCR2CO + NO2  ;
% J<54> : LVR8NO3 = LVR8O + NO2  ;
% 9.16D-13 : LVR8NO3 + OH = LVR8CO + NO2  ;
% J<54> : LVRO6R1NO3 = LVRO6R1O + NO2  ;
% 9.16D-13 : LVRO6R1NO3 + OH = LVRO6R1CO + NO2  ;
% J<56> : LVCR7NO3 = LVCR7O + NO2  ;
% 7.30D-13 : LVCR7NO3 + OH = LVCR7CO + NO2  ;
% J<53> : LVDR6NO3 = LVDR6O + NO2  ;
% 7.30D-13 : LVDR6NO3 + OH = LVDR6CO + NO2  ;
% J<53> : LVROO6R6NO3 = LVROO6R6O + NO2  ;
% 7.30D-13 : LVROO6R6NO3 + OH = LVROO6R6CO + NO2  ;
% J<54> : LVR9NO3 = LVR9O + NO2  ;
% 9.16D-13 : LVR9NO3 + OH = LVR9CO + NO2  ;
% J<54> : LVROO6R7NO3 = LVROO6R7O + NO2  ;
% 9.16D-13 : LVROO6R7NO3 + OH = LVROO6R7CO + NO2  ;
% J<55> : LVROO6R1NO3 = LVROO6R1O + NO2  ;
% J<54> : LVR2NO3 = LVR2O + NO2  ;
% 9.16D-13 : LVR2NO3 + OH = LVR2CO + NO2  ;
% J<54> : LVDR8NO3 = LVDR8O + NO2  ;
% 9.16D-13 : LVDR8NO3 + OH = LVDR8CO + NO2  ;
% J<54> : LVCR9NO3 = LVCR9O + NO2  ;
% 9.16D-13 : LVCR9NO3 + OH = LVCR9CO + NO2  ;
% J<55> : LVDR9NO3 = LVDR9O + NO2  ;
% J<55> : LVDR10NO3 = LVDR10O + NO2  ;
% 9.16D-13 : LVRO5R2NO3 + OH = LVRO5R2CO + NO2  ;
% J<54> : LVDR3NO3 = LVDR3O + NO2  ;
% 9.16D-13 : LVDR3NO3 + OH = LVDR3CO + NO2  ;
% J<53> : LVROO6R14NO3 = LVROO6R14O + NO2  ;
% 7.30D-13 : LVROO6R14NO3 + OH = LVROO6R14CO + NO2  ;
% J<54> : LVROO6R3NO3 = LVROO6R3O + NO2  ;
% 9.16D-13 : LVROO6R3NO3 + OH = LVROO6R3CO + NO2  ;
% J<55> : LVRO6R3NO3 = LVRO6R3O + NO2  ;
% J<54> : LVRO5R4NO3 = LVRO5R4O + NO2  ;
% 9.16D-13 : LVRO5R4NO3 + OH = LVRO5R4CO + NO2  ;
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* DILUTION
*********************
% DILUTE : ACETOL =  ;
% DILUTE : BPINAO2 =  ;
% DILUTE : BPINBO2 =  ;
% DILUTE : BPINCO =  ;
% DILUTE : BPINCO2 =  ;
% DILUTE : BPINENE =  ;
% DILUTE : C3DIALOO =  ;
% DILUTE : CH2OHCOOO =  ;
% DILUTE : CH3COCH3 =  ;
% DILUTE : FORMACET =  ;
% DILUTE : GLYOX =  ;
% DILUTE : HCHO =  ;
% DILUTE : HCOCH2CHO =  ;
% DILUTE : HMACR =  ;
% DILUTE : HO2 =  ;
% DILUTE : LVBPINYLc =  ;
% DILUTE : LVBPINYLd =  ;
% DILUTE : LVCR10NO3 =  ;
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% DILUTE : CH3O2 =  ;


* Number of species: 322
* Number of reactions : 963
```