Chemical equation set

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Table 1: Reaction added to the MECCA submodel in EMAC .

reaction	rate coefficient
$OH + C_4H_{10} \rightarrow HCHO + 0.4365\ CH_3CHO + 0.4365\ PA + 4.254\ PINKO_2$	$1.69 \times 10^{-17} * T^2 * e^{(145/T)}$
$CL + C_4H_{10} \rightarrow HCHO + 0.3575\ CH_3CHO + 0.3575\ PA + 4.57\ PINKO_2$	2.18×10^{-10}
$NO_3 + C_4H_{10} \rightarrow HCHO + 0.4365\ CH_3CHO + 0.4365\ PA + 4.2524\ PINKO_2$	$2.76 \times 10^{-12} * e^{(-3279/T)}$
$OH + IC_4H_{10} \rightarrow .206\ PrO_2 + .794\ CH_3COCH_3 + .794\ CH_3O_2 + 1.206\ PINKO_2$	$1.16 \times 10^{-17} * T^2 * e^{(225/T)}$
$CL + IC_4H_{10} \rightarrow 0.564\ PrO_2 + 0.436\ CH_3COCH_3 + 0.436\ CH_3O_2 + 1.564\ PINKO_2$	1.43×10^{-10}
$NO_3 + IC_4H_{10} \rightarrow 0.206\ PrO_2 + 0.794\ CH_3COCH_3 + 0.794\ CH_3O_2 + 1.206\ PINKO_2$	1.06×10^{-16}
$OH + C_5H_{12} \rightarrow 1.4765\ HCHO + 0.349\ CH_3CHO + 0.1745\ EtO_2 + 6.302\ PINKO_2$	$2.44 \times 10^{-17} * T^2 * e^{(183/T)}$
$CL + C_5H_{12} \rightarrow 1.67\ HCHO + 0.220\ CH_3CHO + 0.11\ EtO_2 + 6.56\ PINKO_2$	2.80×10^{-10}
$NO_3 + C_5H_{12} \rightarrow 1.4765\ HCHO + 0.349\ CH_3CHO + 0.1745\ EtO_2 + 6.302\ PINKO_2$	8.7×10^{-17}
$OH + IC_5H_{12} \rightarrow 0.087\ HCHO + 0.384\ CH3CHO + 0.297\ PrO_2 + 0.616\ CH_3COCH_3 + 0.616\ EtO_2 + 1.435\ PINKO_2$	3.70×10^{-12}
$CL + IC_5H_{12} \rightarrow 0.408\ HCHO + 0.750\ CH3CHO + 0.342\ PrO_2 + 0.250\ CH_3COCH_3 + 0.250\ EtO_2 + 3.04\ PINKO_2$	2.20×10^{-10}
$NO_3 + IC_5H_{12} \rightarrow 0.087\ HCHO + 0.384\ CH3CHO + 0.297\ PrO_2 + 0.616\ CH_3COCH_3 + 0.616\ EtO_2 + 1.435\ PINKO_2$	1.62×10^{-16}
$PINKO_2 + NO \rightarrow 0.95\ NO_2 + 0.475\ HO_2 + 0.475\ PINK + 0.05\ PINKNO_3$	$\left(2.54 * e^{(360./T)} + 8.10 * e^{(270./T)}\right) \times 10^{-12}/2$
$PINKO_2 + CH_3O_2 \rightarrow 0.5\ HO_2 + 0.335\ CH_3OH + 0.665\ HCHO + 0.335\ HO_2$	$2. \times 10^{-12}$
$PINKO_2 + HO_2 \rightarrow PINKOOH$	$\left(4.30 * e^{(1040./T)} + 2.91 * e^{(1300./T)}\right) \times 10^{-13}/2$
$PINK + OH \rightarrow CO_2$	2×10^{-11}
$PINK + hv \rightarrow HO_2$	J-CH3CHO
$PINKNO_3 + OH \rightarrow NO_2$	$5. \times 10^{-12}$
$PINKNO_3 + hv \rightarrow NO_2$	3.7*J-PAN
$PINKOOH + hv \rightarrow OH + 0.5\ HO_2$	J-CH3OOH
$PINKOOH + OH \rightarrow PINKO_2$	$1.90 \times 10^{-12} * e^{(190./T)}$
$PINKOOH + OH \rightarrow OH$	$2. \times 10^{-11}$

[a] Saunders et al. (1997a)
[b] Saunders et al. (1997b)
[c] Atkinson and Arey (2003), branching ratio like the OH reaction
[d] as general aldehyde
[e] photolysis scale with PAN photolysis rate
[f] photolysis scale with CH_3OOH photolysis rate
[g] representative for the H-abstraction of these peroxides
[h] average between the reactions of the two different peroxides isomers

References

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