Table S2: Species Glossary of Species Important at Low Temperature for MCH

In mchxqiy:
x = location of OOH group  
(Note: q means OOH group) 
y = location of radical site j
Note: for mch2xqy and mch3xqy, position 5 and 6 must be defined to account for additional isomers:

(4-membered and 8-membered ring RO₂ isomerizations were not included due to comparatively low reaction rate constants)
Species Glossary of Species Important at Low Temperature for MCH (Continued)

- **chxj3ch2q** (not included)

- **c7ene-one** (lumped species representing 3 species above)

- **c7enej-one** (lumped radical species of c7ene-one)
  - Radical site on formyl group

- **c7enej-one** (lumped radical species of c7ene-one)
  - Radical site on allylic position

- **mchyo23** (a lumped species representing all the 1,2-epoxides in methylcyclohexane)

- **mchyo24** (a lumped species representing all the 1,3-epoxides in methylcyclohexane)

- **mchyo25** (a lumped species representing all the 1,4-epoxides in methylcyclohexane)

- **mche** (lumped species representing all three isomers of methyl-cyclohexene)
Species Glossary of Species Important at Low Temperature for MCH (Continued)
Species Glossary of Species Important at Low Temperature for MCH (Continued)

- chxdch2
- chxyco-2
- c6h11cho1
- chxdo

- ccocccc.
- cc.ccccco
- ic6h12cho-5
- ic6h12cho-2

- ic6h12cho-3
- ic6h12cho-4
- mchje
  (A lumped species for the methylcyclohexene radical)
- mchde
  (A lumped species for the methylcyclohexadiene)
Species Glossary of Species Important at Low Temperature for MCH (Continued)

mchjde
(A lumped species for the methylcyclohexadiene radical)

\[ \text{mchjde} \]

\[ \text{c*ccc*cc.c} \]

\[ \text{cc.c*cccco} \]

\[ \text{mch2q3qj} \]

\[ \text{mch2o3q} \]

\[ \text{mch2o3oj} \]

\[ \text{mch2o3o} \]

\[ \text{mch2q1qj} \]

\[ \text{mch2o1q} \]
Species Glossary of Species Important at Low Temperature for MCH (Continued)
Species Glossary of Species Important at Low Temperature for MCH (Continued)

\[
\begin{align*}
\text{mch2o5oj} & \quad \text{mch2o5o} & \quad \text{mch2q6qj} \\
\text{mch2o6q} & \quad \text{mch2o6oj} & \quad \text{mch2o6o (not included)}
\end{align*}
\]