# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC56



This data sheet last evaluated: February 2009; last change in preferred values: August 2002.

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**$HO_2 + CH_3OCH_2O_2 \rightarrow O_2 + CH_3OCH_2OOH$ (1)**

**$\rightarrow O_2 + CH_3OCHO + H_2O$ (2)**

Rate coefficient data ($k = k_1 + k_2$)

| $k$ / cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| Branching Ratios<br>$k_1/k = 0.53 \pm 0.08$<br>$k_2/k = 0.40 \pm 0.04$ | 295 | Wallington et al., 1993 | P-FTIR (a) |

## Comments

(a) $HO_2$ and $CH_3OCH_2O_2$ radicals were generated from the steady-state photolysis of $Cl_2$ in the presence of $CH_3OH$-$CH_3OCH_3$-$O_2$ mixtures at a total pressure of 930 mbar (700 Torr). Branching ratios were derived from FTIR analyses of $CH_3OCHO$ and $CH_3OCH_2OOH$ products, which accounted for (93 ± 12)% of the $CH_3OCH_3$ loss.

## Preferred Values

| Parameter | Value | T/K |
|---|---|---|
| $k_1/k$ | 0.6 | 298 |
| $k_2/k$ | 0.4 | 298 |
| *Reliability* | | |
| $\Delta k_1/k$ | ± 0.1 | 298 |
| $\Delta k_2/k$ | ± 0.1 | 298 |

*Comments on Preferred Values*

The preferred values of the branching ratios are based on the sole study of Wallington et al. (1993). The participation of channels (1) and (2) at room temperature is analogous to that reported for the reaction between $HO_2$ and the structurally-related $HOCH_2O_2$ radical; but contrasts with that generally observed for unsubstituted $RO_2$ radicals, for which the hydroperoxide-forming channels dominate. It has been proposed by Wallington et al. (1993) that channel (2) proceeds through a six-member transition state similar to that suggested by Russell (1957) to explain the molecular products from the interactions of $RO_2$ radicals. It is noted that evidence for a further, minor channel of the $HO_2$ + $HOCH_2O_2$ reaction, forming HO + $HOCH_2O$ + $O_2$, has recently been reported (Jenkin et al., 2007), and studies are required to investigate whether an analogous channel forming HO + $CH_3OCH_2O$ + $O_2$ exists for the reaction of $HO_2$ with $CH_3OCH_2O_2$.

There have been no kinetics studies of the reaction. However, Jenkin et al. (1993) inferred a value

of $k \approx 10^{-11}$ $cm^3$ $molecule^{-1}$ $s^{-1}$ from the steady state concentration of $HO_2$ radicals formed from the self-reaction of $CH_3OCH_2O_2$ radicals in molecular modulation experiments.

## References


Jenkin, M. E., Hayman, G. D., Wallington, T. J., Hurley, M. D., Ball, J. C., Nielsen, O. J. and Ellermann, T.: J. Phys. Chem., 97, 11712, 1993.

Jenkin, M. E., Hurley, M. D. and Wallington, T. J.: Phys. Chem. Chem. Phys., 9, 3149, 2007.

Russell, G.: J. Am. Chem. Soc., 79, 3871, 1957.

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