IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_7

This data sheet last evaluated: June 2008; last change in preferred values: not applicable.

$CH_3OCH_2O + O_2 \rightarrow CH_3OCHO + HO_2$ **(1)**

$CH_3OCH_2O + M \rightarrow CH_3OCHO + H + M$ **(2)**

Rate coefficient data

$k_1 \cdot k_2^{-1}$/ cm^3 molecule^{-1}	Temp./K	Reference	Technique/ Comments
$k_1[O_2] \approx k_2$(1 bar, air)	295	Jenkin et al., 1993	RR (a)

Comments

(a) Steady-state photolysis of Cl_2-CH_3OCH_3-O_2-N_2 mixtures at pressures of 13.3 mbar to 1000 mbar (10 Torr to 760 Torr) with long-path FTIR analyses, and molecular modulation studies of similar reactant mixtures with UV absorption monitoring of $CH_3OCH_2O_2$ radicals. In both systems, kinetic treatments indicate that reactions (1) and (2) were competing under the conditions of the experiments.

Preferred Values

No quantitative recommendations.

Comments on Preferred Values

Although the results listed above for the reactions of the CH_3OCH_2O radical are not quantitative, for the purposes of atmospheric modelling studies it is recommended that the above qualitative information on the ratios k_1/k_2 be used to decide if one or the other of the alkoxy radical reaction pathways predominates, or if both pathways should be considered. An estimate for the lifetime of CH_3OCH_2O with respect to channel (2) has been obtained by Song et al. (2005). An average value of $k_2 = 8000 \pm 7000$ s^{-1} was calculated based on *ab initio* G3MP2 calculations of the PES and variational transition state calculations of the rate constant, compared to 3000 s^{-1} obtained by Jenkin et al. (1993).

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.

Song, X., Hou, H. and Wang, B.: Phys. Chem. Chem. Phys. 7, 3980, 2005.