IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC71

This data sheet last evaluated: June 2009.

HO + $HOCH_2CH_2OH$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.36 \pm 0.13) \times 10^{-11}$	296 ± 2	Aschmann and Atkinson, 1998	RR (a, b)
$(1.54 \pm 0.14) \times 10^{-11}$	296 ± 2	Aschmann and Atkinson, 1998	RR (a, c)

Comments

(a) Relative rate method carried out at atmospheric pressure of air. HO radicals were generated by the photolysis of CH_3ONO-NO-air + 1,2-ethanediol + *m*-xylene + cyclohexane mixtures at wavelengths > 300 nm. The concentrations of $HOCH_2CH_2OH$, cyclohexane and *m*-xylene (the reference compounds) were measured during the experiments by gas chromatography with flame ionization detection (GC-FID). The measured rate coefficient ratios of k(HO + $HOCH_2CH_2OH$)/k(HO + cyclohexane) = 1.96 ± 0.18 and k(HO + $HOCH_2CH_2OH$)/k(HO + *m*-xylene) = 0.667 ± 0.062 are placed on an absolute basis using k(HO + cyclohexane) = 6.92×10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K (Calvert et al., 2008) and k(HO + *m*-xylene) = 2.31×10^{-11} cm^3 molecule^{-1} s^{-1} (Calvert et al., 2002).

(b) Relative to HO + cyclohexane

(c) Relative to HO + *m*-xylene

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.45×10^{-11}	298
Reliability		
$\Delta \log k$	± 0.20	298

Comments on Preferred Values

The preferred value is an average of the relative rate coefficients of Aschmann and Atkinson (1998) obtained with two reference compounds. In the presence of O_2, the reaction of OH with 1,2-ethandiol is expected to produce glycolaldehyde ($HOCH_2CHO$) with a formation yield of unity:

$HO + HOCH_2CH_2OH \rightarrow H_2O + HOCH_2CHOH$

$HOCH_2CHOH + O_2 \rightarrow HOCH_2CHO + HO_2$

References

Aschmann, S. M., and Atkinson, R.: Int. J. Chem. Kinet., 30, 533, 1998.

Calvert, J. G., Atkinson, R., Becker, K. H., Kamens, R. M., Seinfeld, J. H., Wallington, T. J., and Yarwood, G.: The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons, Oxford University Press, New York, NY, 2002.

Calvert, J. G., Derwent, R. G., Orlando, J. J., Tyndall, G. S., and Wallington, T. J.: Mechanisms of Atmospheric Oxidation of Alkanes, Oxford University Press, New York, NY, 2008.