IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC28

This data sheet last evaluated: 2nd August 2007; no revision of preferred values.

HO + $CH_3CH(OH)CH_2CH_3$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
(8.58 ± 0.49) x 10^{-12}	296 ± 2	Chew and Atkinson, 1996	RR (a)
(8.80 ± 0.14) x 10^{-12}	297 ± 3	Baxley and Wells, 1998	RR (b,c)
(7.57 ± 0.44) x 10^{-12}	297 ± 3	Baxley and Wells, 1998	RR (b,d)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO in air, and the concentrations of 2-butanol and cyclohexane (the reference compound) were measured by GC. The measured rate coefficient ratio of k(HO + 2-butanol)/k(HO + cyclohexane) = 1.24 ± 0.07 is placed on an absolute basis by use of a rate coefficient of k(HO + cyclohexane) = 6.92 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K (Atkinson, 2003).

(b) HO radicals were generated by the photolysis of CH_3ONO in air, and the concentrations of 2-butanol and *n*-nonane and *n*-dodecane (the reference compounds) were measured by GC. The measured rate coefficient ratios of k(HO + 2-butanol)/k(HO + *n*-nonane) and k(HO + 2-butanol)/k(HO + *n*-dodecane) are placed on an absolute basis by use of rate coefficients at 297 K of k(HO + *n*-nonane) = 9.69 x 10^{-12} cm^3 molecule^{-1} s^{-1} and k(HO + *n*-dodecane) = 1.32 x 10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson, 2003).

(c) Relative to HO + *n*-nonane.

(d) Relative to HO + *n*-dodecane.

Preferred Values

k = 8.7 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.15$ at 298 K.

Comments on Preferred Values

The preferred value is based on the relative rate coefficient of Chew and Atkinson (1996) and that of Baxley and Wells (1998) relative to HO + *n*-nonane, which are in excellent agreement. The rate coefficient of Baxley and Wells (1998) measured relative to that for HO + *n*-

dodecane, while in agreement with the other two rate coefficients (Chew and Atkinson, 1996; Baxley and Wells, 1998), is more uncertain because of the small data-base for HO + *n*-dodecane (Atkinson, 2003), and hence this rate coefficient is not used in the evaluation.

References

Atkinson, R.: Atmos. Chem. Phys. 3, 2233, 2003.
Baxley, J. S. and Wells, J. R.: Int. J. Chem. Kinet. 30, 745, 1998.
Chew, A. A. and Atkinson, R.: J. Geophys. Res. 101, 28649, 1996.