IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM9

This data sheet last evaluated November 2008; last change in preferred values November 2008.

HO + 1,2-dihydroxy-4-methylbenzene → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.60 \pm 0.08) \times 10^{-10}$	300 ± 5	Olariu et al., 2000	RR (a,b)
$(1.52 \pm 0.04) \times 10^{-10}$	300 ± 5	Olariu et al., 2000	RR (a,c)
$(1.50 \pm 0.03) \times 10^{-10}$	300 ± 5	Olariu et al., 2000	RR (a,d)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO. Experiments were carried out in a 1080 L chamber at 1.013 bar of air. The concentrations of 1,2-dihydroxy-4-methylbenzene and isoprene, 1,3-butadiene or *trans*-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,2-dihydroxy-4-methylbenzene were measured and taken into account in the data analysis, and these contributed ~30% of the 1,2-dihydroxy-4-methylbenzene loss rate due to HO radical reaction during the experiments. The measured rate coefficient ratios of k(HO + 1,2-dihydroxy-4-methylbenzene)/k(HO + isoprene) = 1.61 ± 0.072, k(HO + 1,2-dihydroxy-4-methylbenzene)/k(HO + 1,3-butadiene) = 2.31 ± 0.048 and k(HO + 1,2-dihydroxy-4-methylbenzene)/k(HO + *trans*-2-butene) = 2.37 ± 0.047 are placed on an absolute basis by use of rate coefficients at 300 K of k(HO + isoprene) = 9.91×10^{-11} cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation), k(HO + 1,3-butadiene) = 6.59×10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003) and k(HO + *trans*-2-butene) = 6.32×10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003).
(b) Relative to k(HO + isoprene).
(c) Relative to k(HO + 1,3-butadiene).
(d) Relative to k(HO + *trans*-2-butene).

Preferred Values

$k = 1.5 \times 10^{-10}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

Comments on Preferred Values

The three rate coefficients measured by Olariu et al. (2000) at 300 ± 5 K using a relative rate method with three different reference compounds are in excellent agreement. The 298 K preferred

value is an average of the three values of Olariu et al. (2000). The assigned uncertainty reflects the fact that all of the data are from a single study.

References

Atkinson, R. and Arey, J.: Chem. Rev., 103, 4605, 2003.
IUPAC: http://iupac.pole-ether.fr, 2013
Olariu, R. I., Barnes, I., Becker, K. H. and Klotz, B.: Int. J. Chem. Kinet., 32, 696, 2000.