IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM14

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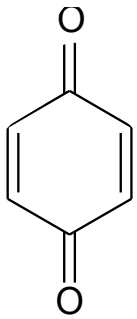
This data sheet last evaluated November 2008; last change in preferred values November 2008.

HO + 1,4-Benzoquinone → products



Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(4.66 \pm 0.10) \times 10^{-12}$	300 ± 5	Olariu et al., 2000	RR (a,b)
$(4.55 \pm 0.14) \times 10^{-12}$	300 ± 5	Olariu et al., 2000	RR (a,c)
$(4.61 \pm 0.13) \times 10^{-12}$	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 1,4-benzoquinone and isoprene, 1,3-butadiene or *trans*-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,4-benzoquinone were measured and taken into account in the data analysis, and these contributed ~30% of the 1,4-benzoquinone loss rate due to HO radical reaction during the experiments. The measured rate coefficient ratios of k(HO + 1,4-benzoquinone)/k(HO + isoprene) = 0.047 ± 0.001, k(HO + 1,4-benzoquinone)/k(HO + 1,3-butadiene) = 0.069 ± 0.002 and k(HO + 1,4-benzoquinone)/k(HO + *trans*-2-butene) = 0.073 ± 0.002 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

$k = 4.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

Comments on Preferred Values

The 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.