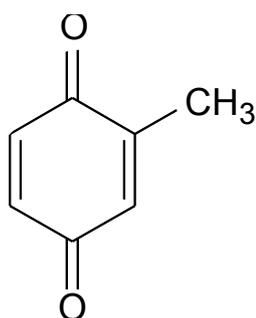


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_AROM15

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

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

HO + methyl-1,4-benzoquinone → products



Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(2.28 \pm 0.10) \times 10^{-11}$	300 ± 5	Olariu et al., 2000	RR (a,b)
$(2.37 \pm 0.07) \times 10^{-11}$	300 ± 5	Olariu et al., 2000	RR (a,c)
$(2.34 \pm 0.07) \times 10^{-11}$	300 ± 5	Olariu et al., 2000	RR (a,d)

Comments

- (a) HO radicals were generated by the photolysis of CH₃ONO. Experiments were carried out in a 1080 L chamber at 1.013 bar of air. The concentrations of methyl-1,4-benzoquinone and isoprene, 1,3-butadiene or *trans*-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of methyl-1,4-benzoquinone were measured and taken into account in the data analysis, and these contributed ~30% of the methyl-1,4-benzoquinone loss rate due to HO radical reaction during the experiments. The measured rate coefficient ratios of $k(\text{HO} + \text{methyl-1,4-benzoquinone})/k(\text{HO} + \text{isoprene}) = 0.23 \pm 0.01$, $k(\text{HO} + \text{methyl-1,4-benzoquinone})/k(\text{HO} + 1,3\text{-butadiene}) = 0.36 \pm 0.01$ and $k(\text{HO} + \text{methyl-1,4-benzoquinone})/k(\text{HO} + \textit{trans}\text{-2-butene}) = 0.37 \pm 0.01$ are placed on an absolute basis by use of rate coefficients at 300 K of $k(\text{HO} + \text{isoprene}) = 9.91 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation), $k(\text{HO} + 1,3\text{-butadiene}) = 6.59 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003) and $k(\text{HO} + \textit{trans}\text{-2-butene}) = 6.32 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).
- (b) Relative to $k(\text{HO} + \text{isoprene})$.
- (c) Relative to $k(\text{HO} + 1,3\text{-butadiene})$.
- (d) Relative to $k(\text{HO} + \textit{trans}\text{-2-butene})$.

Preferred Values

$k = 2.3 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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.