

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_AROM8

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

HO + 1,2-dihydroxy-3-methylbenzene → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(1.90 \pm 0.07) \times 10^{-10}$	300 ± 5	Olariu et al., 2000	RR (a,b)
$(1.99 \pm 0.06) \times 10^{-10}$	300 ± 5	Olariu et al., 2000	RR (a,c)
$(1.99 \pm 0.07) \times 10^{-10}$	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 1,2-dihydroxy-3-methylbenzene and isoprene, 1,3-butadiene or *trans*-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,2-dihydroxy-3-methylbenzene were measured and taken into account in the data analysis, and these contributed ~30% of the 1,2-dihydroxy-3-methylbenzene loss rate due to HO radical reaction during the experiments. The measured rate coefficient ratios of $k(\text{HO} + 1,2\text{-dihydroxy-3-methylbenzene})/k(\text{HO} + \text{isoprene}) = 1.92 \pm 0.07$, $k(\text{HO} + 1,2\text{-dihydroxy-3-methylbenzene})/k(\text{HO} + 1,3\text{-butadiene}) = 3.02 \pm 0.09$ and $k(\text{HO} + 1,2\text{-dihydroxy-3-methylbenzene})/k(\text{HO} + \textit{trans}\text{-2-butene}) = 3.15 \pm 0.1$ 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

$$k = 2.0 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

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

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.

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Olariu, R. I., Barnes, I., Becker, K. H. and Klotz, B.: Int. J. Chem. Kinet., 32, 696, 2000.