IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_AROM8

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

O_3 + 4-methyl-1,2-dihydroxybenzene → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.39 \pm 0.41) \times 10^{-17}$	298 ± 3	Tomas et al., 2003	S-FTIR (a)
Relative Rate Coefficients			
$(2.51 \pm 0.24) \times 10^{-17}$	298 ± 3	Tomas et al., 2003	RR (b,c)
$(2.95 \pm 0.35) \times 10^{-17}$	298 ± 3	Tomas et al., 2003	RR (b,d)

Comments

(a) The disappearance of 4-methyl-1,2-dihydroxybenzene was monitored by FTIR spectroscopy in the presence of excess O_3 in a 1080 L quartz chamber at atmospheric pressure of air. The decay rates of 4-methyl-1,2-dihydroxybenzene to the chamber walls were taken into account in the data analysis.

(b) Relative rate study, with a scavenger (1,2,3- or 1,3,5-trimethylbenzene or *m*-cresol) being present to scavenge HO radicals formed from the O_3 reactions. The concentrations of 4-methyl-1,2-dihydroxybenzene and propene or 1,3-butadiene (the reference compounds) were measured by FTIR spectroscopy. The decay rates of 4-methyl-1,2-dihydroxybenzene to the chamber walls were taken into account in the data analysis. The measured rate coefficient ratios of $k(O_3$ + 4-methyl-1,2-dihydroxybenzene$)/k(O_3$ + propene$) = 2.51 \pm 0.24$ and $k(O_3$ + 4-methyl-1,2-dihydroxybenzene$)/k(O_3$ + 1,3-butadiene$) = 4.68 \pm 0.55$ are placed on an absolute basis by use of rate coefficients at 298 K of $k(O_3$ + propene$) = 1.0 \times 10^{-17}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation) and $k(O_3$ + 1,3-butadiene$) = 6.3 \times 10^{-18}$ cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003).

(c) Relative to propene.

(d) Relative to 1,3-butadiene.

Preferred Values

$k = 2.6 \times 10^{-17}$ 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 Tomas et al. (2003) at 298 K using absolute and relative rate methods (the latter with two reference compounds) are in good agreement. The 298 K preferred value is an average of the three values of Tomas et al. (2003). 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.
Tomas, A., Olariu, R. I., Barnes, I. and Becker, K. H.: Int. J. Chem. Kinet., 35, 223, 2003.