

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_AROM6

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

O₃ + 1,2-dihydroxybenzene (1,2-C₆H₄(OH)₂) → products

Rate coefficient data

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
8.59 × 10 ⁻¹⁸	298 ± 3	Tomas et al., 2003	S-FTIR (a)
<i>Relative Rate Coefficients</i>			
(8.5 ± 0.8) × 10 ⁻¹⁸	298 ± 3	Tomas et al., 2003	RR (b,c)
(1.06 ± 0.14) × 10 ⁻¹⁷	298 ± 3	Tomas et al., 2003	RR (b,d)

Comments

- (a) The disappearance of 1,2-dihydroxybenzene was monitored by FTIR spectroscopy in the presence of excess O₃ in a 1080 L quartz chamber at atmospheric pressure of air. The decay rates of 1,2-dihydroxybenzene to the chamber walls were taken into account in the data analysis. The cited rate coefficient is the average from two experiments.
- (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 O₃ reactions. The concentrations of 1,2-dihydroxybenzene and propene or 1,3-butadiene (the reference compounds) were measured by FTIR spectroscopy. The decay rates of 1,2-dihydroxybenzene to the chamber walls were taken into account in the data analysis. The measured rate coefficient ratios of $k(\text{O}_3 + 1,2\text{-dihydroxybenzene})/k(\text{O}_3 + \text{propene}) = 0.85 \pm 0.08$ and $k(\text{O}_3 + 1,2\text{-dihydroxybenzene})/k(\text{O}_3 + 1,3\text{-butadiene}) = 1.69 \pm 0.22$ are placed on an absolute basis by use of rate coefficients at 298 K of $k(\text{O}_3 + \text{propene}) = 1.0 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation) and $k(\text{O}_3 + 1,3\text{-butadiene}) = 6.3 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).
- (c) Relative to propene.
- (d) Relative to 1,3-butadiene.

Preferred Values

$$k = 9.2 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

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

Comments on Preferred Values

The three rate coefficients measured by 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.

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Tomas, A., Olariu, R. I., Barnes, I. and Becker, K. H.: Int. J. Chem. Kinet., 35, 223, 2003.