

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO₃_AROM9

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

NO₃ + 1,2-dihydroxy-4-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>			
$(1.60 \pm 0.06) \times 10^{-10}$	298 ± 2	Olariu et al., 2004	RR (a)
$(1.35 \pm 0.04) \times 10^{-10}$	296 ± 2	Olariu et al., 2004	RR (b)

Comments

- (a) NO₃ radicals generated by the thermal decomposition of N₂O₅. Experiments were carried out in a 1080 L chamber at 1 bar of air. The concentrations of 1,2-dihydroxy-4-methylbenzene and 2,3-dimethyl-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,2-dihydroxy-4-methylbenzene were measured and taken into account in the data analysis, and these contributed ~40% of the 1,2-dihydroxy-4-methylbenzene loss rate due to NO₃ radical reaction during the experiments. The measured rate coefficient ratio of $k(\text{NO}_3 + 1,2\text{-dihydroxy-4-methylbenzene})/k(\text{NO}_3 + 2,3\text{-dimethyl-2-butene}) = 2.80 \pm 0.10$ is placed on an absolute basis by use of a rate coefficient of $k(\text{NO}_3 + 2,3\text{-dimethyl-2-butene}) = 5.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).
- (b) NO₃ radicals generated by the thermal decomposition of N₂O₅. Experiments were carried out in the ~200 m³ EUPHORE chamber at atmospheric pressure of air. The concentrations of 1,2-dihydroxy-4-methylbenzene and 2,3-dimethyl-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,2-dihydroxy-4-methylbenzene were measured and taken into account in the data analysis, and these contributed ~40% of the 1,2-dihydroxy-4-methylbenzene loss rate due to NO₃ radical reaction during the experiments. The measured rate coefficient ratio of $k(\text{NO}_3 + 1,2\text{-dihydroxy-4-methylbenzene})/k(\text{NO}_3 + 2,3\text{-dimethyl-2-butene}) = 2.36 \pm 0.06$ is placed on an absolute basis by use of a rate coefficient of $k(\text{NO}_3 + 2,3\text{-dimethyl-2-butene}) = 5.72 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).

Preferred Values

$$k = 1.5 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

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

Comments on Preferred Values

The two rate coefficients measured by Olariu et al. (2004) at 296-298 K in two reaction chambers differing in volume by a factor of ~200 using a relative rate method agree to within 20%. The 298 K preferred value is an average of the two values of Olariu et al. (2004). 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.

Olariu, R. I., Bejan, I., Barnes, I., Klotz, B., Becker, K. H. and Wirtz, K.: *Int. J. Chem. Kinet.*, 36, 577, 2004.