IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_AROM7

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

NO_3 + 1,2-dihydroxybenzene (1,2-$C_6H_4(OH)_2$) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(9.03 \pm 0.41) \times 10^{-11}$	298 ± 2	Olariu et al., 2004	RR (a)
$(1.08 \pm 0.07) \times 10^{-10}$	296 ± 2	Olariu et al., 2004	RR (b)

Comments

(a) NO_3 radicals generated by the thermal decomposition of N_2O_5. Experiments were carried out in a 1080 L chamber at 1 bar of air. The concentrations of 1,2-dihydroxybenzene and 2,3-dimethyl-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,2-dihydroxybenzene were measured and taken into account in the data analysis, and these contributed ~40% of the 1,2-dihydroxybenzene loss rate due to NO_3 radical reaction during the experiments. The measured rate coefficient ratio of $k(NO_3 + 1,2\text{-dihydroxybenzene})/k(NO_3 + 2,3\text{-dimethyl-2-butene}) = 1.58 \pm 0.07$ is placed on an absolute basis by use of a rate coefficient of $k(NO_3 + 2,3\text{-dimethyl-2-butene}) = 5.72 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003).

(b) NO_3 radicals generated by the thermal decomposition of N_2O_5. Experiments were carried out in the ~200 m^3 EUPHORE chamber at atmospheric pressure of air. The concentrations of 1,2-dihydroxybenzene and 2,3-dimethyl-2-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses of 1,2-dihydroxybenzene were measured and taken into account in the data analysis, and these contributed ~40% of the 1,2-dihydroxybenzene loss rate due to NO_3 radical reaction during the experiments. The measured rate coefficient ratio of $k(NO_3 + 1,2\text{-dihydroxybenzene})/k(NO_3 + 2,3\text{-dimethyl-2-butene}) = 1.88 \pm 0.11$ is placed on an absolute basis by use of a rate coefficient of $k(NO_3 + 2,3\text{-dimethyl-2-butene}) = 5.72 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003).

Preferred Values

$k = 9.9 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.15$ at 298 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.