IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM11

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

HO + 4-methyl-2-nitrophenol → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(3.53 \pm 0.18) \times 10^{-12}$	296 ± 3	Bejan et al., 2007	RR (a,b)
$(3.60 \pm 0.54) \times 10^{-12}$	296 ± 3	Bejan et al., 2007	RR (a,c)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO. Experiments were carried out in a 1080 L chamber at 1.013 bar of air. The concentrations of 4-methyl-2-nitrophenol and ethene or *n*-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses and photolysis of 4-methyl-2-nitrophenol were measured and taken into account in the data analysis, and these contributed ~50-55% of the total measured 4-methyl-2-nitrophenol loss rate during the experiments. The measured rate coefficient ratios of k(HO + 4-methyl-2-nitrophenol)/k(HO + ethene) = 0.41 ± 0.02 and k(HO + 4-methyl-2-nitrophenol)/k(HO + *n*-butane) = 1.55 ± 0.23 are placed on an absolute basis by use of rate coefficients at 296 K and atmospheric pressure of air of k(HO + ethene) = 8.61×10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson and Arey, 2003) and k(HO + *n*-butane) = 2.32×10^{-12} cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).
(b) Relative to k(HO + ethene).
(c) Relative to k(HO + *n*-butane).

Preferred Values

$k = 3.6 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

Comments on Preferred Values

The rate coefficients measured by Bejan et al. (2007) at 296 ± 3 K using a relative rate method with two different reference compounds are in excellent agreement. The 298 K preferred value is an un-weighted average of the two values of Bejan et al. (2007). The assigned uncertainty reflects the fact that all of the data are from a single study and the need to account for significant wall losses and photolysis of the 4-methyl-2-nitrophenol.

References

Atkinson, R. and Arey, J.: Chem. Rev., 103, 4605, 2003.
IUPAC: http://iupac.pole-ether.fr, 2013.
Bejan, I., Barnes, I., Olariu, R., Zhou, S., Wiesen, P. and Benter, Th.: Phys. Chem. Chem. Phys., 9, 5686, 2007.