IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM12

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

HO + 5-methyl-2-nitrophenol → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(5.77 \pm 0.35) \times 10^{-12}$	296 ± 3	Bejan et al., 2007	RR (a,b)
$(7.60 \pm 1.56) \times 10^{-12}$	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 5-methyl-2-nitrophenol and ethene or *n*-butene (the reference compounds) were measured by FTIR spectroscopy. Wall losses and photolysis of 5-methyl-2-nitrophenol were measured and taken into account in the data analysis, and these contributed 29-33% of the total measured 5-methyl-2-nitrophenol loss rate during the experiments. The measured rate coefficient ratios of k(HO + 5-methyl-2-nitrophenol)/k(HO + ethene) = 0.67 ± 0.04 and k(HO + 5-methyl-2-nitrophenol)/k(HO + *n*-butane) = 3.274 ± 0.67 (the rate coefficient ratio cited in Bejan et al. (2007) is in error (I. Barnes, private communication, 2008)) 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

$k = 6.7 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.2$ 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 reasonable 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 5-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.