IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM26

This datasheet last evaluated: June 2009.

HO + $C_6H_5CH_2OH$ (benzyl alcohol) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(2.75 \pm 0.66) \times 10^{-12}$	297 ± 3	Harrison and Wells, 2009	RR-GC (a, b)
$(2.61 \pm 0.58) \times 10^{-12}$	297 ± 3	Harrison and Wells, 2009	RR-GC (a, c)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO-NO-air mixtures in 1 atmosphere of air at $\lambda > 300$ nm. Experiments were carried out in a ~50-80 liter Teflon chamber, and the concentrations of benzyl alcohol, n-decane and hexanal (the reference compounds) were measured during the experiments by gas chromatography. The measured rate coefficient ratios of k(HO + benzyl alcohol)/k(HO + n-decane) = 2.5 ± 0.6 and k(HO + benzyl alcohol)/k(HO + hexanal) = 0.9 ± 0.2 are placed on an absolute basis using k(HO + n-decane) = 1.1×10^{-11} cm^3 molecule^{-1} s^{-1} and k(HO + hexanal) = 2.9×10^{-11} cm^3 molecule^{-1} s^{-1} (Calvert et al., 2008).
(b) Relative to HO + n-decane
(c) Relative to HO + hexanal

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.7×10^{-11}	298
Reliability		
$\Delta \log k$	± 0.20	298

Comments on Preferred Values

The preferred value is an average of the relative rate coefficients of Harrison and Wells (2009) obtained with two reference compounds. This value is in good agreement with the unpublished absolute measurement of Nolting et al., $k = (2.29 \pm 0.25) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} at 298 K, cited in Atkinson (1989). Hippler et al. (1991) reported $k = 8.3 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at high temperature

(1180-1450 K). This value was derived from a fit to the experimental profiles of stable products in shock-heated benzyl iodide/HNO_3/Ar mixtures.

The reaction proceeds both by H-atom abstraction from the $–CH_2OH$ group and via addition to the aromatic ring. In their mechanistic study, Harrison and Wells (2009) observed benzaldehyde, glyoxal and 4-oxo-pentenal as products of the reaction. Benzaldehyde is produced following hydrogen atom abstraction from $–CH_2OH$ group while glyoxal and 4-oxo-pentenal are expected to be formed following addition of HO radicals to the aromatic ring.

References

Atkinson, R.: J. Phys. Chem. Ref. Data; Monograph 1, 246 pp., 1989.

Calvert, J. G., Derwent, R. G., Orlando, J. J., Tyndall, G. S., and Wallington, T. J.: Mechanisms of Atmospheric Oxidation of Alkanes, Oxford University Press, New York, NY, 2008.

Harrison, J. C., and Wells, J. R.: Atmos. Environ., 43, 798, 2009.

Hippler, H., Reihs, C., and Troe, J.: Symp. Int. Combust. Proc. 23, 37, 1991.