IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM21

This data sheet last evaluated: June 2009.

HO + Furan-2,5-dione → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.36 \pm 0.07) \times 10^{-12}$	296 ± 2	Bierbach et al., 1994	RR-FTIR (a, b)

Comments

(a) HO radicals were generated by the photolysis of H_2O_2 in 1000 mbar of air at λ = 254 nm. Experiments were carried out in a 1080-L quartz-glass chamber, and the concentrations of furan-2,5-dione and n-butane (the reference compound) were measured in situ by long-path FTIR using an optical path length of 492 m and a spectral resolution of 1 cm^{-1}. The measured rate coefficient ratio of k(HO + furan-2,5-dione)/k(HO + n-butane) = 0.58 ± 0.03 is placed on an absolute basis using k(HO + butane) = 2.35×10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).
(b) Relative to HO + n-butane.

Preferred Value

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.4×10^{-12}	298
Reliability		
$\Delta \log k$	± 0.20	298

Comments on Preferred Value

The preferred value is based on the sole study of Bierbach et al. (1994) in 1 bar of air.

Bierbach et al. (1994) conducted a product analysis of the HO-initiated oxidation of furan-2,5-dione (maleic anhydride) using either photolysis of H_2O_2 or CH_3ONO/NO/air as the HO source. CO (20% yield) and HCOOH (3% yield) were observed as reaction products using both sources. Acetylene (5%) was observed only with H_2O_2 as the HO source. CO_2 was reported a major reaction products but could not be quantified. The product IR spectra showed two carbonyl absorptions in the region 1820-1720

cm^{-1} but the identity of the compounds could not be determined. Bierbach et al. (1994) did not find evidence for the formation of PAN or other peroxynitrate type compounds.

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.

Bierbach, A., Barnes, I., Becker, K. H., and Wiesen, E.: Environ. Sci. Technol. 28, 715, 1994.