IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM22

This data sheet last evaluated: June 2009.

HO + $CH_3C(O)CH=CHCHO$ (*cis*/*trans*-4-oxopent-2-enal) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(6.18 \pm 0.23) \times 10^{-11}$	296 ± 2	Bierbach et al., 1994	RR-FTIR (a)

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 cis/trans-4-oxopent-2-enal and propene (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 + 4-oxopent-2-enal)/k(HO + propene) = 2.13 ± 0.08 is placed on an absolute basis using k(HO + propene) = 2.9×10^{-11} cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

Preferred Value

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	6.2×10^{-11}	298
Reliability		
Δ 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.

The reaction proceeds both by H-atom abstraction from the -CHO group and via addition to the double bond. Bierbach et al. (1994) reported that the HO reaction with a mixture of *cis*/*trans*-oxopent-2-enal isomers leading to formation of furan-2,5-dione (maleic anhydride) in a 40% yield which was taken as an indication that the abstraction channel plays an important role. Bierbach et al. (1994) also observed, but were not able to quantify, the formation of glyoxal and methylglyoxal which are expected to be

major products following HO addition to the >C=C< double bond. The formation yield of 5-methyl-3*H*-furanone was reported to be 1%.

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.