

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_AROM19

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HO + *trans*-CHOCH=CHCHO → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> $\geq (2.67 \pm 0.87) \times 10^{-11}$	296 ± 2	Bierbach et al., 1994	RR-FTIR (a, b)

Comments

- (a) HO radicals were generated by the photolysis of H₂O₂ in 1000 mbar of air at $\lambda = 254$ nm. Experiments were carried out in a 1080-L quartz-glass chamber, and the concentrations of *trans*-but-2-enedial 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. Because of difficulties in the analysis of the data caused by *trans/cis* isomerisation, only a lower limit for the rate coefficient ratio could be derived $k(\text{HO} + \text{trans-but-2-enedial})/k(\text{HO} + \text{propene}) \geq 0.92$. This ratio is placed on an absolute basis using $k(\text{HO} + \text{propene}) = 2.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson et al., 2006).
- (b) Relative to HO + propene.

Preferred Value

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$\geq 2 \times 10^{-11}$	298

Comments on Preferred Value

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

The reaction proceeds both by H-atom abstraction from the -CHO groups and via addition to the double bond. In their mechanistic study of the OH reaction with a mixture of *cis/trans*-butenedial isomers, Bierbach et al. (1994) have reported that slightly less than 50% of the reaction proceeds by H-atom abstraction from the aldehyde functional groups of butenedial leading to furan-2,5-dione (maleic anhydride). Glyoxal, expected to be major product of the OH addition, has been also observed as a reaction product but could not be quantified. The formation yield of 3*H*-furan-2-one was reported to be 4%.

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; 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.