# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_AROM18


This data sheet last evaluated: June 2009.

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## HO + *cis*-CHOCH=CHCHO → products

### Rate coefficient data

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | $T$/K | Reference | Technique/ Comments |
|---|---|---|---|
| *Relative Rate Coefficients* | | | |
| $(5.77 \pm 0.12) \times 10^{-11}$ | 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 *cis*-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$^{-1}$. The measured rate coefficient ratio of $k$(HO + *cis*-but-2-enedial)/$k$(HO + propene) = 1.99 ± 0.04 is placed on an absolute basis using $k$(HO + propene) = $2.9 \times 10^{-11}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ (Atkinson et al., 2006).

(b) Relative to HO + propene

### Preferred Values

| Parameter | Value | $T$/K |
|---|---|---|
| $k$ /cm$^3$ molecule$^{-1}$ s$^{-1}$ | $5.8 \times 10^{-11}$ | 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 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.