

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_VOC43

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This data sheet last evaluated: 30th July 2007; no revision of preferred values.

HO + 2-C₄H₉ONO₂ → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(6.4 \pm 1.0) \times 10^{-13}$	299 ± 2	Atkinson et al., 1982	RR (a,b)
$(8.6 \pm 1.5) \times 10^{-13}$	298 ± 2	Atkinson and Aschmann, 1989	RR (a,c)

Comments

- HO radicals were generated by the photolysis of CH₃ONO in one atmosphere of air. The concentrations of 2-butyl nitrate and the reference organic were measured by GC.
- Experiments were carried out in an ~75 liter Teflon chamber, and the data were interpreted as involving concurrent photolysis of 2-butyl nitrate. The measured rate constant ratio of $k(\text{HO} + 2\text{-butyl nitrate})/k(\text{HO} + \text{cyclohexane}) = 0.091 \pm 0.013$ is placed on an absolute basis by use of a rate coefficient of $k(\text{HO} + \text{cyclohexane}) = 7.00 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 299 K (Atkinson, 2003).
- Experiments were carried out in a 6400 liter Teflon chamber, and irradiations were also carried out in the absence of CH₃ONO allowing the photolysis rate to be accurately allowed for in the data analysis. The measured rate coefficient ratio of $k(\text{HO} + 2\text{-butyl nitrate})/k(\text{HO} + \text{cyclohexane}) = 0.123 \pm 0.021$ is placed on an absolute basis by use of a rate coefficient of $k(\text{HO} + \text{cyclohexane}) = 6.97 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K (Atkinson, 2003). These data supersede those of Atkinson et al. (1982).

Preferred Values

$$k = 8.6 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.3 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred value is based on the rate coefficient of Atkinson and Aschmann (1989), which supersedes the earlier study of Atkinson et al. (1982). By analogy with the reaction of the HO radical with 2-propyl nitrate (IUPAC, 2007), the temperature dependence of the rate coefficient at temperatures below 300 K is likely to be small.

References

Atkinson, R.: *Atmos. Chem. Phys.* 3, 2233, 2003.

Atkinson, R. and Aschmann, S. M.: *Int. J. Chem. Kinet.* 21, 1123, 1989.

Atkinson, R., Aschmann, S. M., Carter, W. P. L. and Winer, A. M.: *Int. J. Chem. Kinet.* 14, 919, 1982.

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