

Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO_x_VOC44

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. This data sheet last evaluated: 2nd August 2007; no revision of preferred values.

HO + CH₃C(O)OONO₂ → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$\leq 1.7 \times 10^{-13}$	299 ± 1	Winer et al., 1977	FP-RF
$1.23 \times 10^{-12} \exp[-(651 \pm 229)/T]$	273-297	Wallington et al., 1984	FP-RF
$(1.37 \pm 0.05) \times 10^{-13}$	297 ± 2		
$(7.5 \pm 1.4) \times 10^{-14}$	298	Tsalkani et al., 1988	DF-EPR
$<3.0 \times 10^{-14}$	298	Talukdar et al., 1995	FP/PLP-LIF (a)

Comments

- (a) Experiments were carried out over the temperature range 253-298 K, using pulsed laser photolysis of HONO at 355 nm, pulsed laser photolysis of O₃-H₂O mixtures at 266 nm, or flash photolysis of H₂O at 165-185 nm to generate HO radicals. The measured HO radical decay rates corresponded to rate coefficients in the range $(0.82\text{-}2.50) \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with no obvious dependence on temperature. The measured HO radical decay rates were attributed to the reaction of HO radicals with HCHO impurity, and a conservative upper limit to the rate coefficient k was cited (see table).

Preferred Values

$k < 3 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

Comments on Preferred Values

The preferred upper limit to the 298 K rate coefficient is the upper limit reported by Talukdar et al. (1995) from an extensive and careful study. The higher rate coefficients measured by Wallington et al. (1984) and Tsalkani et al. (1988) were almost certainly due to the presence of reactive impurities.

References

- Talukdar, R. K., Burkholder, J. B., Schmoltner, A.-M., Roberts, J. M., Wilson, R. R. and Ravishankara, A. R.: J. Geophys. Res. 100, 14163, 1995.
Tsalkani, N., Mellouki, A., Poulet, G., Toupance, G. and Le Bras, G.: J. Atmos. Chem. 7, 409, 1988.
Wallington, T. J., Atkinson, R. and Winer, A. M.: Geophys. Res. Lett. 11, 861, 1984.
Winer, A. M., Lloyd, A. C., Darnall, K. R., Atkinson, R. and Pitts Jr., J. N.: Chem. Phys. Lett. 51, 221, 1977.