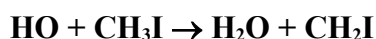


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oIOx1

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: June 2015; last change in preferred values: June 2004.



$$\Delta H^\circ = -63.1 \text{ kJ}\cdot\text{mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$3.1 \times 10^{-12} \exp[-(1119 \pm 205)/T]$	271-423	Brown et al., 1990	DF-RF
$(7.2 \pm 0.7) \times 10^{-14}$	298		
$(1.2 \pm 0.4) \times 10^{-13}$	299	Gilles et al., 1996	PLP-LIF (a)
$(9.9 \pm 2.0) \times 10^{-14}$	298 ± 2	Cotter et al., 2003	DF-RF

Comments

- (a) Derived from the time-concentration profiles of HO radicals monitored by LIF after generation of O(³P) atoms (from 193 nm pulsed laser photolysis of N₂O in N₂) in the presence of varying amounts of CH₃I.

Preferred Values

$$k = 1.0 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k = 4.3 \times 10^{-12} \exp(-1120/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range } 270\text{-}430 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.2 \text{ at } 298 \text{ K.}$$

$$\Delta(E/R) = \pm 500 \text{ K.}$$

Comments on Preferred Values

The room temperature rate coefficients of Brown et al. (1990), Gilles et al. (1996) and Cotter et al. (2003) are in reasonable agreement, and the preferred 298 K rate coefficient is an average of the room temperature rate coefficients from these three studies. The temperature dependence obtained by Brown et al. (1990), the only temperature-dependent study to date, is accepted and the pre-exponential factor is adjusted to fit the 298 K preferred value.

References

- Brown, A. C., Canosa-Mas, C. E. and Wayne, R. P.: Atmos. Environ. 24A, 361, 1990.
Cotter, E. S. N., Canosa-Mas, C. E., Manners, C. R., Wayne, R. P. and Shallcross, D. E.: Atmos. Environ. 37, 1125, 2003.

Gilles, M. K., Turnipseed, A. A., Talukdar, R. K., Rudich, Y., Villalta, P. W., Huey, L. G., Burkholder, J. B. and Ravishankara, A. R.: J. Phys. Chem. 100, 14005, 1996.