

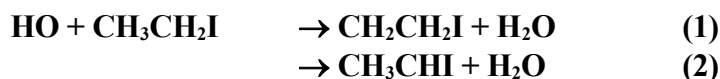
IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

Data Sheet oIOx4; VII.A4.1

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Rate coefficient data ($k = k_1 + k_2$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$5.55 \times 10^{-12} \exp[-(830 \pm 90)/T]$	297-372	Zhang et al. (2012)	FP-RF (a)
$(3.24 \pm 0.08) \times 10^{-13}$	298		
<i>Relative Rate Coefficients</i>			
$(5.5 \pm 1.0) \times 10^{-13}$	298	Cotter et al. (2003)	DF-RF (b)

Comments

- (a) HO radicals were generated by the VUV flash photolysis of H₂O in 188 Torr (250 mbar) of helium diluent. HO radicals were monitored using resonance fluorescence at 308 nm.
- (b) HO radicals were generated by the reaction of H atoms with NO₂ in 1.5 or 5.0 Torr (2.0 or 6.7 mbar) of helium diluent at 298 ± 2 K. There was no discernable effect of total pressure over the range studied. It is possible that the measured rate coefficient is an overestimation of $k(\text{HO} + \text{C}_2\text{H}_5\text{I})$ because of additional loss of HO radicals via reaction with products of the HO + C₂H₅I reaction. While secondary chemistry should manifest itself in curvature of the first order ($\ln([\text{HO}]_{t_0}/[\text{HO}]_t)$ versus time) plots, Cotter et al. (2003) calculated that such curvature would not be discernable given the data scatter. Cotter et al. (2003) estimated that correction of the rate coefficient for possible additional loss of HO radicals via secondary reactions would lower the rate coefficient to $5.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	3.4×10^{-13}	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$5.65 \times 10^{-11} \exp(-841/T)$	290-380
<i>Reliability</i>		
$\Delta \log k$	0.1	298

Comments on Preferred Values

The rate coefficient at 298 K reported by Cotter et al. (2003) is significantly larger than that reported by Zhang et al. (2012). It is unclear to what extent the value reported by Cotter et al. (2003) needs correcting to account for possible additional loss of HO radicals via reaction with products of the HO + C₂H₅I reaction. Hence, the value reported by Cotter et al. (2003) is not inconsistent with results

from Zhang et al. (2012). The recommendation is based upon a fit of the Arrhenius expression to the data from Zhang et al. (2012).

References

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

Zhang, S., Strekowski, R.S., Monod, A., Bosland, L., and Zetzsch, C.: J. Phys. Chem. A, 116, 9497, 2012.

