IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation
Data Sheet oIOx4; VII.A4.1

This datasheet last evaluated: June 2014; last change in preferred values: June 2014

$$HO + CH_3CH_2I \rightarrow CH_2CH_2I + H_2O \quad (1)$$
$$\rightarrow CH_3CHI + H_2O \quad (2)$$

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

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

Comments

(a) HO radicals were generated by the VUV flash photolysis of H_2O 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 NO_2 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 $k(HO+C_2H_5I)$ because of additional loss of HO radicals via reaction with products of the $HO+C_2H_5I$ reaction. While secondary chemistry should manifest itself in curvature of the first order ($\ln([HO]_{to}/[HO]_t$ versus time) plots, Cotter et al. (2003) calculated that such curvature would be 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 5.5×10^{-13} cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	3.4×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	$5.65 \times 10^{-11} \exp(-841/T)$	290-380
Reliability		
$\Delta \log k$	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 addition loss of HO radicals via reaction with products of the HO + C_2H_5I 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.