

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO<sub>x</sub>\_VOC70

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### HO + (CH<sub>3</sub>)<sub>3</sub>COH → products

#### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$T/\text{K}$	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(3.3 \pm 1.6) \times 10^{-12} \exp[-(310 \pm 150)/T]$	240-440	Wallington et al., 1988	FP-RF (a)
$(1.07 \pm 0.08) \times 10^{-12}$	298		
$(8.1 \pm 1.7) \times 10^{-13}$	298	Saunders et al., 1994	DF-LIF (b)
$(2.66 \pm 0.48) \times 10^{-12} \exp[-(270 \pm 130)/T]$	253-372	Téton et al., 1996	PLP-LIF (c)
$(1.08 \pm 0.10) \times 10^{-12}$	298		
<i>Relative Rate Coefficients</i>			
$(1.08 \pm 0.07) \times 10^{-12}$	295 ± 2	Wu et al., 2003	RR (d, e)

#### Comments

- (a) HO radicals were generated by the vacuum ultraviolet ( $\lambda \geq 165$  nm) photolysis of H<sub>2</sub>O and monitored as function of time under pseudo-first order conditions by resonance fluorescence.
- (b) HO radicals were generated by the H + NO<sub>2</sub> reaction and monitored under pseudo-first order conditions by laser induced fluorescence.
- (c) HO radicals were generated by the photolysis of H<sub>2</sub>O<sub>2</sub> and their concentration measured by pulsed laser induced fluorescence.
- (d) HO radicals were generated by the photolysis of H<sub>2</sub>O<sub>2</sub> in 1 atmosphere of air at 254 nm. Experiments were carried out in a ~100 liter Teflon chamber, and the concentrations of t-butyl alcohol and propane (the reference organic) were measured by GC-FID. The measured rate coefficient ratio of  $k(\text{HO} + (\text{CH}_3)_3\text{COH})/k(\text{HO} + \text{propane})$  is placed on an absolute basis using  $k(\text{HO} + \text{propane}) = 1.05 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 295 K (Atkinson et al., 2006).
- (e) Relative to HO + propane

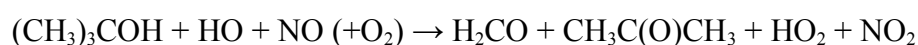
#### Preferred Values

Parameter	Value	$T/\text{K}$
$k/\text{molecule}^{-1} \text{ s}^{-1}$	$1.1 \times 10^{-12} \text{ cm}^3$	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.6 \times 10^{-12} \exp(-121/T)$	240-314
<i>Reliability</i>		
$\Delta \log k$	± 0.08	298
$\Delta E/R$	± 75	

### *Comments on Preferred Values*

The rate coefficient values obtained by Wallington et al. (1988), Téton et al. (1996) and Wu et al. (2003) near 298 K are in very good agreement. The room temperature value of Saunders et al. (1994) is ~25% lower than the others. The Arrhenius plots of the data of Wallington et al. (1988) and Téton et al. (1996) show curvature, fitting the expression  $k = B + C \exp(-D/T)$  to the rate coefficients reported by these authors gives  $k = 9.57 \times 10^{-13} + 5.65 \times 10^{-11} \exp(-1836/T)$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> over the temperature range 240-440 K. For atmospheric purposes, a fit to the data below 314 K of Wallington et al., Téton et al., and Wu et al. yields  $k = 1.6 \times 10^{-12} \exp(-121/T)$ , giving  $k = 1.1 \times 10^{-12}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 298 K.

The reaction of HO radicals with 2-methyl-2-propanol proceeds mainly by H-atom from CH<sub>3</sub>-group. Under atmospheric conditions and in the presence of NO, the main degradation products expected are formaldehyde and acetone (Japar et al., 1990):



### **References**

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