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$$HO + CH_3CH_2Br \rightarrow CH_2CH_2Br + H_2O \quad (1)$$
$$\rightarrow CH_3CHBr + H_2O \quad (2)$$

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

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.77 \pm 0.34) \times 10^{-12} \exp[-(1344\pm86)/T)]$	292-366	Qiu et al. (1992)	DF-RF (a)
3.05×10^{-13}	298		
$1.7 \times 10^{-13}\ T^{0.5} \exp(-641/T)$	233-422	Herndon et al. (2001)	PLP-LIF (b)
3.29×10^{-13}	297		
Relative Rate Coefficients			
$(2.18 \pm 0.07) \times 10^{-13}$	300	Donaghy et al. (1993)	RR (c)

Comments

(a) HO radicals were produced by the reaction of F atoms with H_2O in 2-3 Torr (2.7-4.0 mbar) of argon diluent gas. The value given at 298 K above is the average of the measurements reported by Qiu et al. (1992).
(b) HO radicals were produced by either the photolysis of HONO at 355 nm (third harmonic Nd:YAG laser) or the photolysis of H_2O_2 at 248 nm (KrF eximer laser) in approximately 100 Torr (133 mbar) of helium diluent. The value given at 296 K above is the average of the measurements reported by Herndon et al. (2001).
(c) HO radicals were produced by the photolysis of CH_3ONO in one atmosphere pressure of air. Ethane was used as the reference compound and a rate coefficient ratio of $k(HO+C_2H_5Br)/k(HO+C_2H_6) = 0.885 \pm 0.030$ was reported. Using $k(HO+C_2H_6) = 6.9 \times 10^{-12} \exp(-1000/T)$ (Atkinson et al., 2006) gives $k(HO+C_2H_5Br) = (2.18 \pm 0.07) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	3.3×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	$2.25 \times 10^{-12} \exp(-576/T)$	230-300
Reliability		
$\Delta \log k$	0.15	298
$\Delta E/R$	± 300	

Comments on Preferred Values

The absolute rate coefficients of Qiu et al. (1992) and Herndon et al. (2001) are in reasonable agreement over the temperature range over which measurements were conducted. In contrast, the

rate coefficient reported in the relative rate study of Donaghy et al. (1993) is significantly lower than those reported by Qiu et al. (1992) and Herndon et al. (2001). The temperature dependence reported by Qiu et al. (1992) is substantially greater than that reported by Herndon et al. (2001). However, the factor of two difference between the reported activation energies is misleading as the rate coefficients at the highest and lowest temperature investigated by Qiu et al. (1992) only differ by about 15% from those reported by Herndon et al. (2001). Fitting the three parameter equation $k = CT^2 \exp(-D/T)$ to the data from Qiu et al. (1992) and Herndon et al. (2001) gives $k = 7.12 \times 10^{-18}$ $T^2 \exp(-193/T)$ cm^3 $molecule^{-1}$ s^{-1}. Taking an average of the rate coefficients reported by Qiu et al. (1992) and Herndon et al. (2001) at 296-298 K gives our recommendation of 3.26×10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K. Fitting the Arrhenius expression to this data and that at lower temperatures reported by Herndon et al. (2001) gives $k = 2.25 \times 10^{-12} \exp(-576/T)$ cm^3 $molecule^{-1}$ s^{-1} which is recommended over the range 230-300 K.

References

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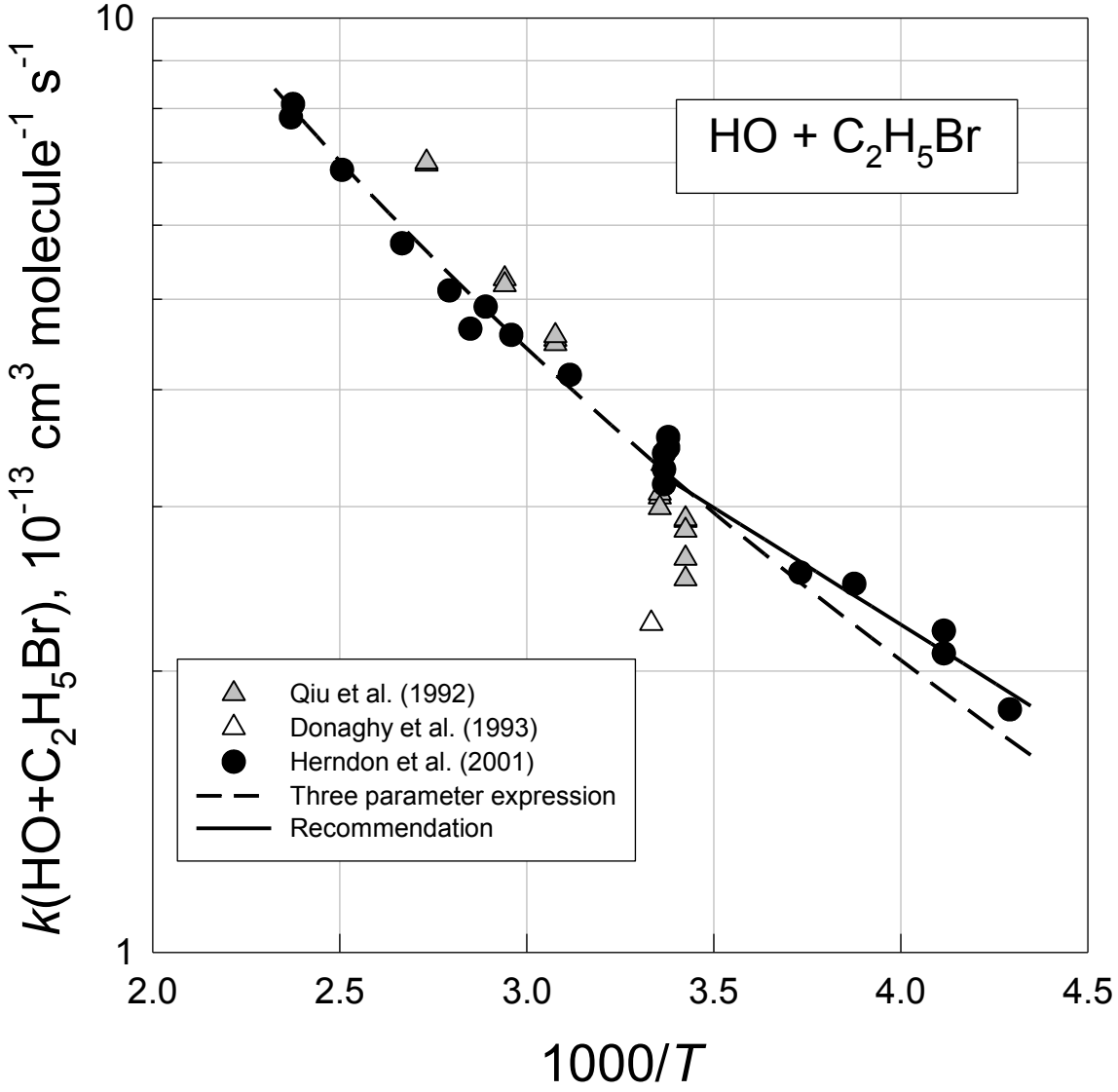
HO + C2H5Br
Qiu et al. (1992)
Donaghy et al. (1993)
Herndon et al. (2001)
Three parameter expression
Recommendation
k(HO+C2H5Br), 10-13 cm3 molecule-1 s-1
1000/T
10
1
2.0
2.5
3.0
3.5
4.0
4.5