IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx_VOC4

This data sheet updated: 12th December 2007 (with no revision of the preferred values).

$$HO + C_2H_6 \rightarrow H_2O + C_2H_5$$

$\Delta H° = -74.1$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.90 \pm 0.60) \times 10^{-13}$	296	Howard and Evenson, 1976	DF-LMR
$(2.6 \pm 0.4) \times 10^{-13}$	298	Leu, 1979	DF-RF
8.0×10^{-14}	238	Margitan and Watson, 1982	PLP-RF
$1.43 \times 10^{-14}\ T^{1.05} \exp(-911/T)$	297-800	Tully et al., 1983	FP-RF
$(2.59 \pm 0.21) \times 10^{-13}$	297		
$1.80 \times 10^{-11} \exp[-(1240 \pm 110)/T]$	240-295	Smith et al., 1984	FP-RF
$(2.63 \pm 0.10) \times 10^{-13}$	295		
2.75×10^{-13}	295	Devolder et al., 1984	DF-RF
$(2.67 \pm 0.40) \times 10^{-13}$	295 ± 2	Baulch et al., 1985	DF-RF
$8.51 \times 10^{-18}\ T^{2.06} \exp(-430/T)$	293-705	Tully et al., 1986	PLP-LIF
$(2.39 \pm 0.10) \times 10^{-13}$	292.5		
$(1.27 \pm 0.08) \times 10^{-13}$	248	Stachnik et al., 1986	PLP-RA
$(1.29 \pm 0.09) \times 10^{-13}$	248		
$(2.51 \pm 0.06) \times 10^{-13}$	297		
$(2.50 \pm 0.06) \times 10^{-13}$	297		
$(2.77 \pm 0.3) \times 10^{-13}$	296 ± 2	Bourmada et al., 1987	DF-RF
$8.4 \times 10^{-12} \exp[-(1050 \pm 100)/T]$	226-363	Wallington et al., 1987	FP-RF
$(2.30 \pm 0.26) \times 10^{-13}$	296		
$(2.61 \pm 0.13) \times 10^{-13}$	296	Zabarnick et al., 1988	PLP-LIF
$(2.38 \pm 0.16) \times 10^{-13}$	297 ± 2	Abbatt et al., 1990	DF-LIF
$(1.54 \pm 0.24) \times 10^{-11}$	1225 ± 16	Bott and Cohen, 1991	SH-RA
$1.03 \times 10^{-11} \exp[-(1108 \pm 40)/T]$	231-377	Talukdar et al., 1994	PLP-LIF
$(2.43 \pm 0.13) \times 10^{-13}$	298		
8.37×10^{-12}	974 ± 16	Koffend and Cohen, 1996	SH-RA
$(2.55 \pm 0.3) \times 10^{-13}$	300	Donahue et al., 1996	DF-LIF
$(2.59 \pm 0.08) \times 10^{-13}$	300	Donahue et al., 1998	DF-LIF
$(3.55 \pm 0.11) \times 10^{-13}$	325		
$(3.90 \pm 0.12) \times 10^{-13}$	340		
$(4.38 \pm 0.23) \times 10^{-13}$	360		
$(5.61 \pm 0.17) \times 10^{-13}$	375		
$(6.04 \pm 0.18) \times 10^{-13}$	390		
$(2.69 \pm 0.27) \times 10^{-14}$	180	Clarke et al., 1998	DF-LIF
$(3.77 \pm 0.04) \times 10^{-14}$	190		
$(4.54 \pm 0.25) \times 10^{-14}$	200		
$(6.51 \pm 0.07) \times 10^{-14}$	213		
$(8.08 \pm 0.12) \times 10^{-14}$	225		

$(9.67 \pm 0.18) \times 10^{-14}$	238
$(1.251 \pm 0.014) \times 10^{-13}$	250
$(1.640 \pm 0.018) \times 10^{-13}$	265
$(2.081 \pm 0.016) \times 10^{-13}$	280
$(2.515 \pm 0.021) \times 10^{-13}$	295
$(2.953 \pm 0.050) \times 10^{-13}$	310
$(3.464 \pm 0.037) \times 10^{-13}$	325
$(3.744 \pm 0.038) \times 10^{-13}$	340
$(4.637 \pm 0.164) \times 10^{-13}$	360

Preferred Values

$k = 2.4 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 6.9 \times 10^{-12} \exp(-1000/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 200-300 K.

Reliability

$\Delta \log k = \pm 0.08$ at 298 K.
$\Delta(E/R) = \pm 100$ K.

Comments on Preferred Values

The preferred values were obtained by using the absolute rate coefficient data of Smith et al. (1984), Tully et al. (1986) (this study being judged to supersede that of Tully et al., 1983), Stachnick et al. (1986), Wallington et al. (1987), Abbatt et al. (1990), Bott and Cohen (1991), Talukdar et al. (1994), Koffend and Cohen (1996), Donahue et al. (1996, 1998) and Clarke et al. (1998). The absolute rate coefficients used in the evaluation (Smith et al., 1984; Tully et al., 1986; Stachnik et al., 1986; Wallington et al., 1987; Abbatt et al., 1990; Bott and Cohen, 1991; Talukdar et al., 1994; Koffend and Cohen, 1996; Donahue et al., 1996; Donahue et al., 1998; Clarke et al., 1998) were fitted to the three-parameter equation $k = CT^2 \exp(-D/T)$, resulting in $k = 1.49 \times 10^{-17} T^2 \exp(-499/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 180-1230 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 250 K and is derived from the three-parameter equation with $A = C e^2 T^2$ and $B = D + 2T$. The preferred Arrhenius expression predicts rate coefficients at 180 K and 190 K which agree to within 6% with those measured by Clarke et al. (1998).

The absolute rate coefficients of Howard and Evenson (1976), Leu (1979), Margitan and Watson (1982), Devolder et al. (1984), Baulch et al. (1985), Bourmada et al. (1987), Zabarnick et al. (1988) and Schiffman et al. (1991) (at room temperature, the precise temperature not being specified), which are not used in the evaluation of the rate coefficient, are in good agreement with the preferred values, as are the relative rate coefficients of Baulch et al. (1983), Edney et al. (1986) and Finlayson-Pitts et al. (1993).

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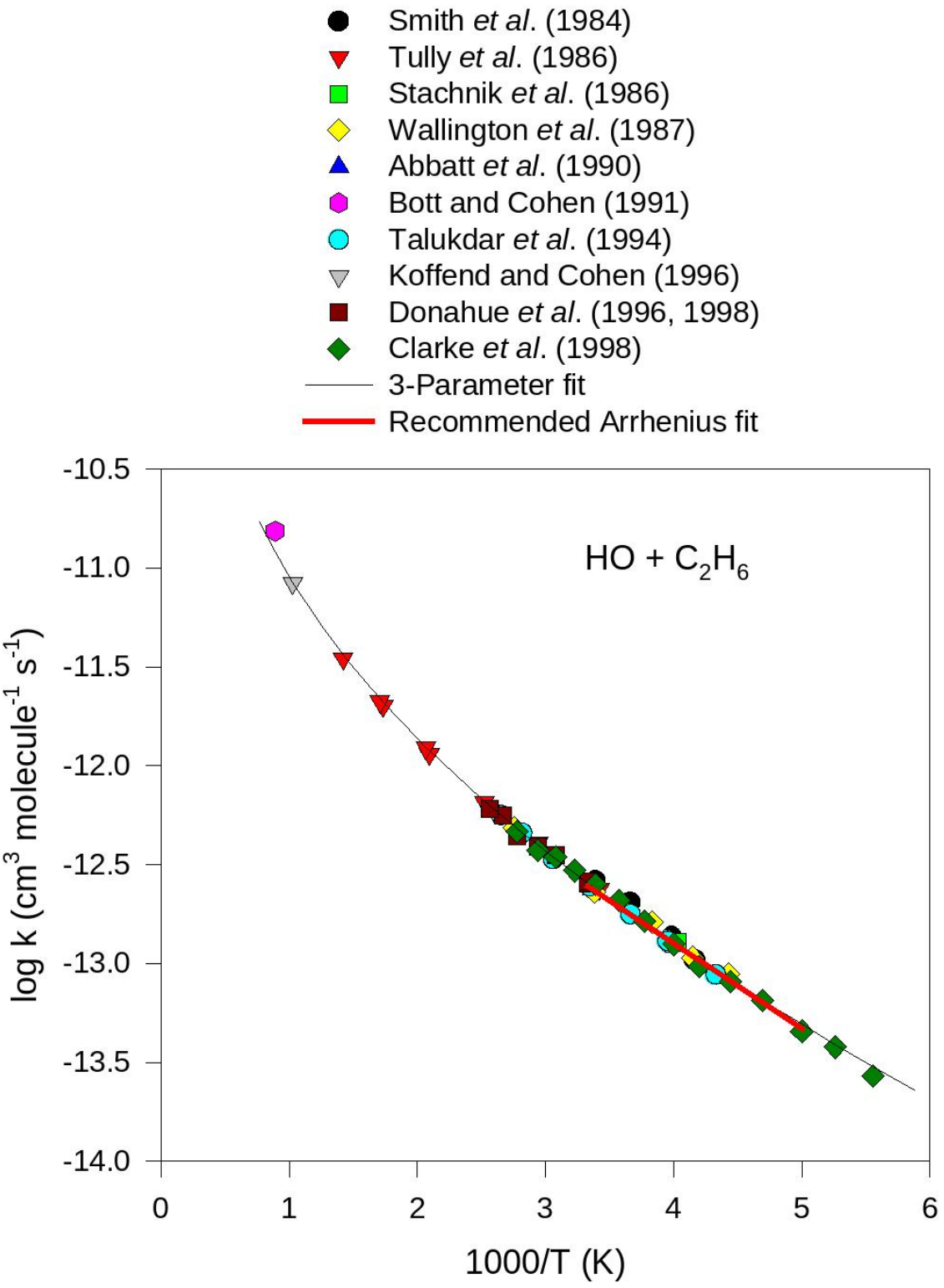
Smith et al. (1984)
Tully et al. (1986)
Stachnik et al. (1986)
Wallington et al. (1987)
Abbatt et al. (1990)
Bott and Cohen (1991)
Talukdar et al. (1994)
Koffend and Cohen (1996)
Donahue et al. (1996, 1998)
Clarke et al. (1998)
3-Parameter fit
Recommended Arrhenius fit
HO + C2H6
log k (cm3 molecule-1 s-1)
-10.5
-11.0
-11.5
-12.0
-12.5
-13.0
-13.5
-14.0
0
1
2
3
4
5
6
1000/T (K)