IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx48

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$HO + CH_3CF_2Cl$ (HCFC-142b) $\rightarrow H_2O + CH_2CF_2Cl$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.83 \pm 0.42) \times 10^{-15}$	296	Howard and Evenson, 1976	DF-LMR
$1.15 \times 10^{-12} \exp[-(1748 \pm 30)/T]$	273-375	Watson et al., 1977	FP-RF
$(3.22 \pm 0.48) \times 10^{-15}$	298		
$1.8 \times 10^{-12} \exp[-(1790 \pm 150)/T]$	293-373	Handwerk and Zellner, 1978	FP-RA
$(3.7 \pm 0.7) \times 10^{-15}$	293		
$3.3 \times 10^{-12} \exp[-(1800 \pm 300)/T]$	293-417	Clyne and Holt, 1979	DF-RF
$(6.7 \pm 1.3) \times 10^{-15}$	298		
$(4.63 \pm 1.73) \times 10^{-15}$	297	Paraskevopoulos et al., 1981	FP-RA
$9.8 \times 10^{-13} \exp[-(1660 \pm 200)/T]$	270-400	Liu et al., 1990	FP-RF
$(4.02 \pm 1.0) \times 10^{-15}$	298		
$2.6 \times 10^{-13} \exp[-(1230 \pm 250)/T]$	231-423	Brown et al., 1990	DF-RF
$(3.7 \pm 1.4) \times 10^{-15}$	303		
$1.14 \times 10^{-12} \exp[-(1750 \pm 75)/T]$	223-374	Gierczak et al., 1991	DF-LMR/FP-LIF (a)
$(2.95 \pm 0.25) \times 10^{-15}$	298		
$(2.45 \pm 0.31) \times 10^{-15}$	270	Zhang et al., 1992	FP-RF
$(2.6 \pm 0.4) \times 10^{-15}$	293	Mörs et al., 1996	PLP-A
$2.05 \times 10^{-30} T^{6.01} \exp[(308 \pm 522)/T]$	295-808	Fang et al., 1997	PLP-LIF
$(3.77 \pm 0.43) \times 10^{-15}$	295		
Relative Rate Coefficients			
3.5×10^{-15}	298	Cox et al., 1976	RR (b)

Comments

(a) Experiments were carried out over the temperature range 223-427 K.

(b) HO radicals were generated by the photolysis of HONO-air mixtures at 1.013 bar pressure. Relative rate coefficients were obtained from measurements of the rates of NO formation as a function of the HONO and organic concentrations. Based on the effect of CH_3CF_2Cl on NO formation and a rate coefficient for the reaction of HO radicals with CH_4 of 6.4×10^{-15} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al., 2006), the rate coefficient cited in the table is obtained

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	3.0 x 10^{-15}	298
k /cm^3 molecule^{-1} s^{-1}	8.5 x 10^{-13} exp(-1685/T)	220-300
Reliability		
$\Delta \log k$	$\pm$ 0.10	298
$\Delta(E/R)$	$\pm$ 200	220-300

Comments on Preferred Values

The rate coefficients obtained exhibit a large degree of scatter, especially at temperatures ≤305 K. In particular, the rate coefficients of Clyne and Holt (1979) and Brown et al. (1990) and, to a lesser extent, those of Handwerk and Zellner (1978), Paraskevopoulos et al. (1981), Liu et al. (1990), Zhang et al. (1992) and Fang et al. (1997) at room temperature and below are higher than those of Howard and Evenson (1976), Watson et al. (1977), Gierczak et al. (1991) and Mörs et al. (1996). Accordingly, the absolute rate coefficients of Howard and Evenson (1976), Watson et al. (1977), Gierczak et al. (1991) and Mörs et al. (1996) have been fitted to the three parameter equation $k = CT^2 \exp(-D/T)$, resulting in $k = 1.77 \times 10^{-18}\ T^2 \exp(-1174/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 223-427 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 255 K and is obtained from the three parameter equation with $A = C\ e^2\ T^2$ and $B = D + 2T$.

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Subcommittee for Gas Kinetic Data Evaluation, http://iupac.pole-ether.fr

Brown, A. C., Canosa-Mas, C. E., Parr, A. D. and Wayne, R. P.: Atmos. Environ., 24A, 2499, 1990.

Clyne, M. A. A. and Holt, P. M.: J. Chem. Soc. Faraday Trans. 2, 75, 582, 1979.

Cox, R. A., Derwent, R. G., Eggleton, A. E. J. and Lovelock, J. E.: Atmos. Environ., 10, 305, 1976.

Fang, T. D., Taylor, P. H., Dellinger, B., Ehlers, C. J. and Berry, R. J.: J. Phys. Chem. A, 101, 5758, 1997.

Gierczak, T., Talukdar, R., Vaghjiani, G. L., Lovejoy, E. R. and Ravishankara, A. R.: J. Geophys. Res., 96, 5001, 1991.

Handwerk, V. and Zellner, R.: Ber. Bunsenges. Phys. Chem., 82, 1161, 1978.

Howard, C. J. and Evenson, K. M.: J. Chem. Phys., 64, 4303, 1976.

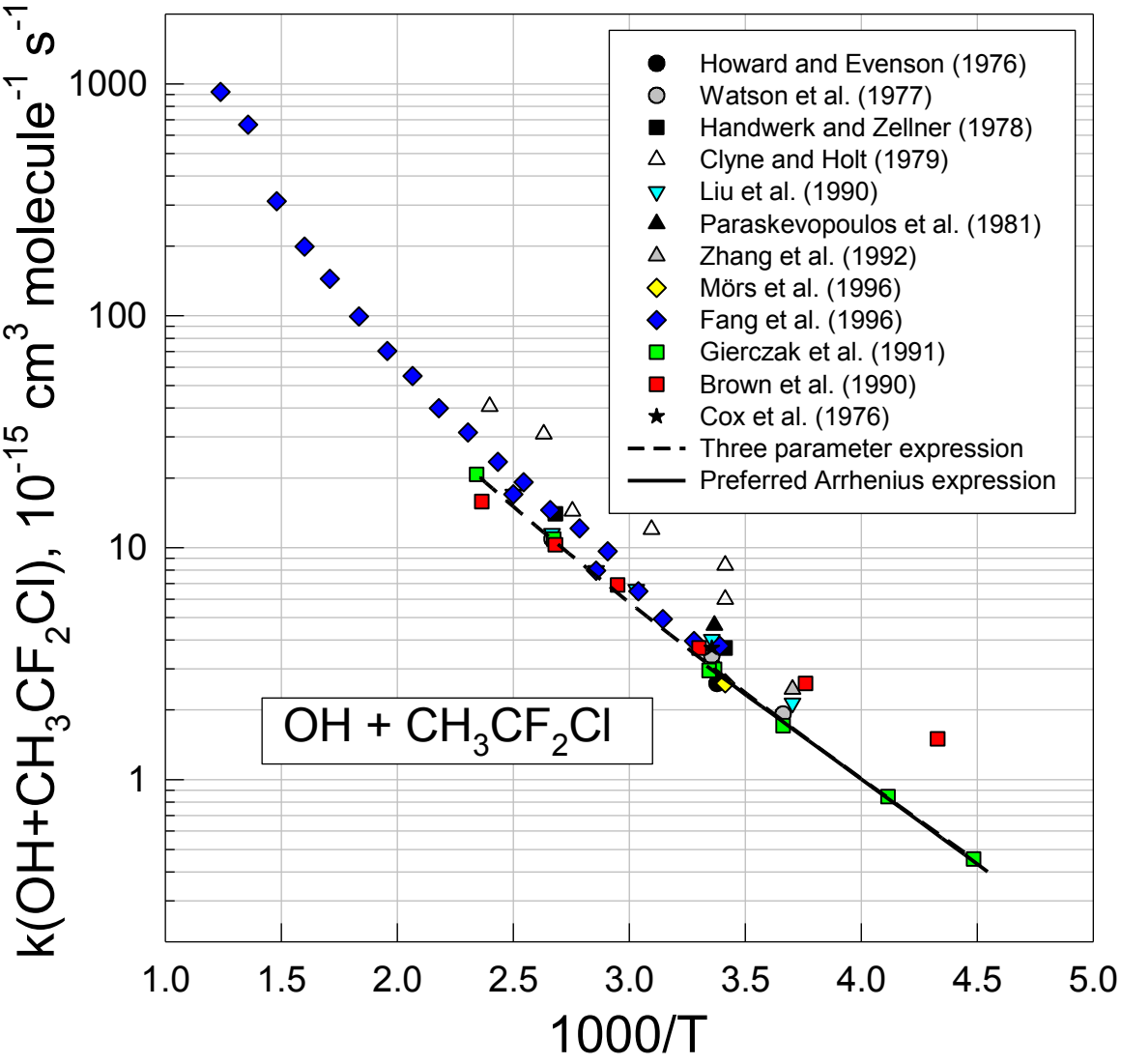
Liu, R., Huie, R. E. and Kurylo, M. J.: J. Phys. Chem., 94, 3247, 1990.

Mörs, V., Hoffmann, A., Malms, W. and Zellner, R.: Ber. Bunsenges. Phys. Chem., 100, 540, 1996.

Paraskevopoulos, G., Singleton, D. L. and Irwin, R. S.: J. Phys. Chem., 85, 561, 1981.

Watson, R. T., Machado, G., Conaway, B., Wagner, S. and Davis, D. D.: J. Phys. Chem., 81, 256, 1977.

Zhang, Z., Huie, R. E. and Kurylo, M. J.: J. Phys. Chem., 96, 1533, 1992.


k(OH+CH3CF2Cl), 10-15 cm3 molecule-1 s-1
1000
100
10
1
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
1000/T
OH + CH3CF2Cl
Howard and Evenson (1976)
Watson et al. (1977)
Handwerk and Zellner (1978)
Clyne and Holt (1979)
Liu et al. (1990)
Paraskevopoulos et al. (1981)
Zhang et al. (1992)
Mörs et al. (1996)
Fang et al. (1996)
Gierczak et al. (1991)
Brown et al. (1990)
Cox et al. (1976)
Three parameter expression
Preferred Arrhenius expression