IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oClOx88; VII.A2.3

This datasheet last evaluated: June 2015; last change in preferred values: June 2009.

$$HO + CH_3CHCl_2 \rightarrow CH_2CHCl_2 + H_2O \quad (1)$$
$$\rightarrow CH_3CCl_2 + H_2O \quad (2)$$

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

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.6 \pm 0.6) \times 10^{-13}$	296	Howard and Evenson (1976)	DF-LMR (a)
$(8.29 \pm 0.36) \times 10^{-14} (T/300)^{2.67} \exp(387 \pm 18)/T$	294-800	Jiang et al. (1992)	PLP-LIF (b)
$(2.82 \pm 0.14) \times 10^{-13}$	294		

Comments

(a) HO radicals were generated by the reaction of H atoms with NO_2 in 0.1-1.0 kPa (0.7-7 Torr) of helium diluent.

(b) HO radicals were produced by the 193 nm photolysis of N_2O to give $O(^1D)$ atoms in the presence of H_2O vapor in 740 ± 10 Torr (986 ± 13 mbar) of helium diluent.

Preferred Values

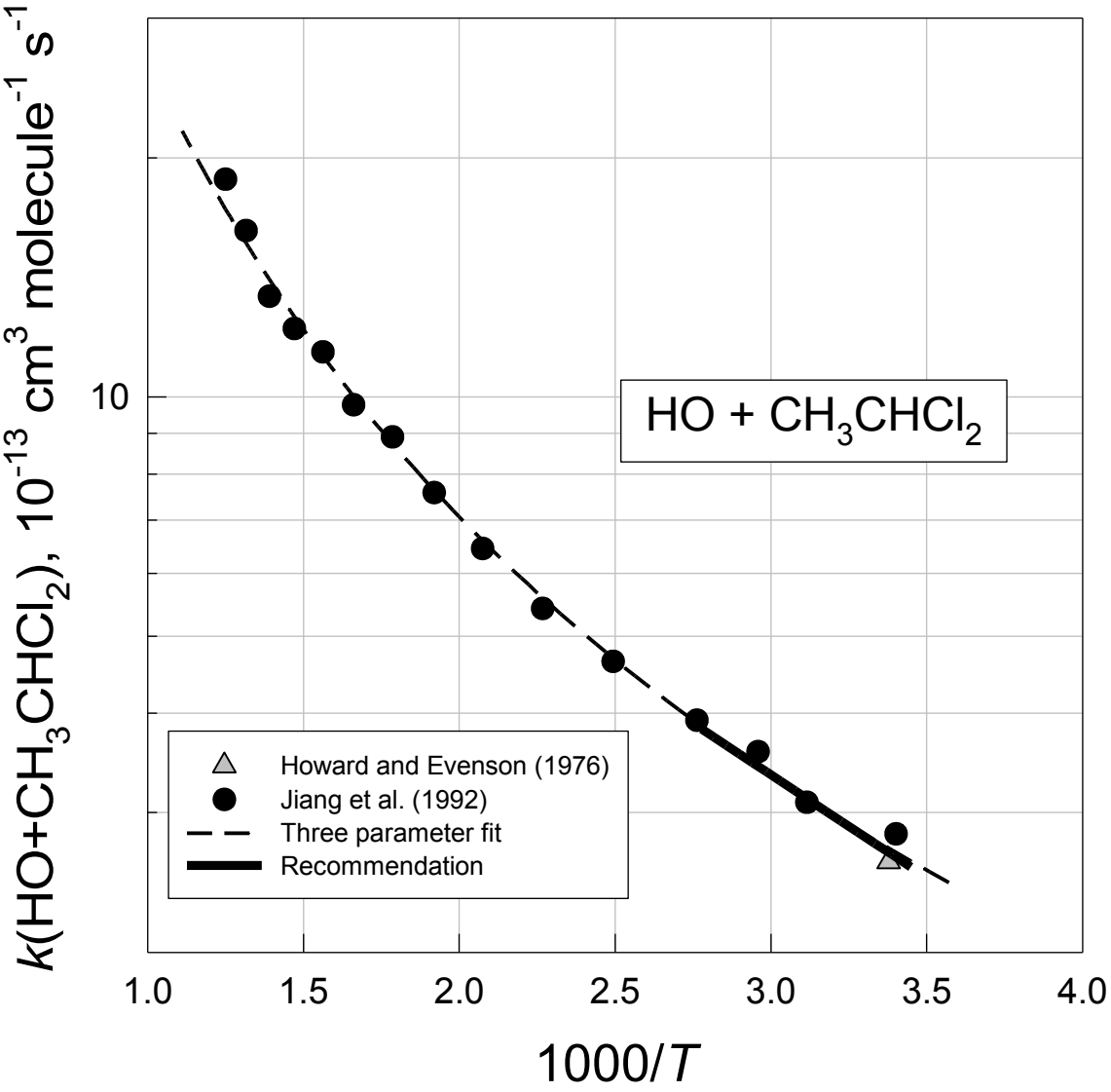
Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.7×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	$2.0 \times 10^{-12} \exp(-596/T)$	290-370
Reliability		
$\Delta \log k$	0.1	298
$\Delta E/R$	± 300	

Comments on Preferred Values

The rate coefficients of Howard and Evenson (1976) and Jiang et al. (1992) at room temperature are in excellent agreement. Fitting the three parameter equation $k = CT^2 \exp(-D/T)$ to the data from Howard and Evenson (1976) and Jiang et al. (1992) gives $k = 2.49 \times 10^{-18} T^2 \exp(64/T)$ cm^3 molecule^{-1} s^{-1}. Centering this expression at 330 K with $A = C\,e^2\,T^2$ and $B = D + 2T$ gives $k = 2.00 \cdot 10^{-12}$ exp(-596/T) cm^3 molecule^{-1} s^{-1}.

References

Howard, C. J., and Evenson, K. M.: J. Chem. Phys., 64, 4303, 1976.
Jiang, Z., Taylor, P.H., and Dellinger, B.: J. Phys. Chem., 96, 8964, 1992.


k(HO+CH_3CHCl_2), 10^{-13} cm^3 molecule^{-1} s^{-1}
10
HO + CH_3CHCl_2
Howard and Evenson (1976)
Jiang et al. (1992)
Three parameter fit
Recommendation
1.0
1.5
2.0
2.5
3.0
3.5
4.0
1000/T