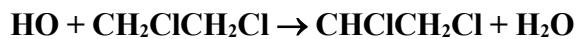


# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx87; VII.A2.2

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This datasheet last evaluated: June 2014; last change in preferred values: June 2009.



## Rate coefficient data ( $k$ )

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.2 \pm 0.5) \times 10^{-13}$	296	Howard and Evenson (1976)	DF-LMR (a)
$4.08 \times 10^{-12} (T/300)^{1.0} \exp[-(825 \pm 88/T)]$	292-775	Taylor et al. (1991)	PLP-LIF (b)
$(2.48 \pm 0.38) \times 10^{-13}$	292		
$1.05 \times 10^{-11} \exp[-(1141 \pm 107)/T]$	292-363	Qiu et al (1992)	DF-RF (c)
$2.14 \times 10^{-13}$	295		
<i>Relative Rate Coefficients</i>			
$(2.50 \pm 0.54) \times 10^{-13}$	297	Arnts et al. (1989)	RR (d)

## Comments

- (a) HO radicals were generated by the reaction of H atoms with NO<sub>2</sub> in 0.1-1.0 kPa (0.7-7 Torr) of helium diluent.
- (b) HO radicals were produced by the 193 nm (ArF eximer laser) photolysis of N<sub>2</sub>O to produce O(<sup>1</sup>D) atoms in the presence of H<sub>2</sub>O in 730-750 Torr (973-1000 mbar) of helium diluent.
- (c) HO radicals were produced by the reaction of F atoms with H<sub>2</sub>O in 2-3 Torr (2.7-4.0 mbar) of argon diluent gas.
- (d) The rate coefficient ratio  $k(\text{HO}+\text{CH}_2\text{ClCH}_2\text{Cl})/k(\text{HO}+\text{C}_2\text{H}_6) = 1.02 \pm 0.22$  was placed on an absolute basis using  $k(\text{HO}+\text{C}_2\text{H}_6) = 1.49 \times 10^{-17} T^2 \exp(-499/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (Atkinson et al., 2006).

## Preferred Values

Parameter	Value	T/K
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2.4 \times 10^{-13}$	298
$k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$8.69 \times 10^{-12} \exp(-1070/T)$	290-360
<i>Reliability</i>		
$\Delta \log k$	0.08	298
$\Delta E/R$	$\pm 200$	

## Comments on Preferred Values

The rate coefficients of Howard and Evenson (1976), Arnts et al. (1989), Taylor et al. (1991), and Qiu et al. (1992) are in good agreement. Fitting the three parameter equation  $k = CT^2 \exp(-D/T)$  to the data from Howard and Evenson (1976), Arnts et al. (1989), Taylor et al. (1991), and Qiu et al. (1992) gives  $k = 1.08 \times 10^{-17} T^2 \exp(-410/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . Centering this expression at 330 K with A = C e<sup>2</sup> T<sup>2</sup> and B = D + 2T gives  $k = 8.69 \times 10^{-12} \exp(-1070/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .

### References

- Arnts, R. R., Seila, R. L., and Bufalini, J. J.: J. Air Pollut. Control Assoc., 39, 453, 1989.  
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>.  
Herndon, S. C., Gierczak, T., Talukdar, R. K., and Ravishankara, A. R.: Phys. Chem. Chem. Phys., 3, 4529, 2001.  
Howard, C. J., and Evenson, K. M.: J. Chem. Phys., 64, 4303, 1976.  
Qiu, L.X., Shi, S.H., Xing, S.B., and Chen, X.G.: J. Phys. Chem., 96, 685, 1992.  
Taylor, P.H., McCarron, S., and Dellinger, B.: Chem. Phys. Lett., 177, 27, 1991.

