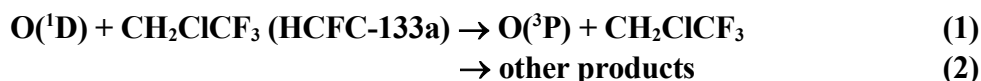


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.79 oClOx5

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 8, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>. This data sheet last evaluated: June 2015; last change in preferred values: November 2003.



$$\Delta H^\circ(1) = -190 \text{ kJ mol}^{-1}$$

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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(1.20 \pm 0.06) \times 10^{-10}$	298	Warren et al., 1991	PLP-RF
<i>Branching Ratios</i>			
$k_1/k = 0.20 \pm 0.05$	298	Warren et al., 1991	PLP-RF (a)
<i>Relative Rate Coefficients</i>			
$k_2 = (1.50 \pm 0.35) \times 10^{-10}$	297	Green and Wayne, 1976	RR (b)

Comments

- (a) Branching ratio was determined from the ratio of the $\text{O}(^3\text{P})$ yield from $\text{O}(^1\text{D}) + \text{CH}_2\text{ClCF}_3$ relative to that for $\text{O}(^1\text{D}) + \text{N}_2$.
- (b) $\text{O}(^1\text{D})$ produced by photolysis of NO_2 at 229 nm. $\Delta(\text{CH}_2\text{ClCF}_3)/\Delta(\text{N}_2\text{O})$ monitored by IR absorption spectroscopy. Measured rate coefficient ratio of $(k_2/k(\text{O}(^1\text{D}) + \text{N}_2\text{O})) = 1.3 \pm 0.3$ is placed on an absolute basis using $k(\text{O}(^1\text{D}) + \text{N}_2\text{O}) = 1.16 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current evaluation). The cited rate coefficient refers to chemical reaction only and does not include physical quenching.

Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	1.2×10^{-10}	298
k_1/k	0.20	298
<i>Reliability</i>		
$\Delta \log k$	± 0.3	298
$\Delta(k_1/k)$	± 0.1	298

Comments on Preferred Values

The preferred value of k and the preferred value of the branching ratio k_1/k are based on the results of Warren et al. (1991). In these experiments, only $\text{O}(^3\text{P})$ was monitored and therefore no

direct information relating to the products of the chemical reaction of $O(^1D) + CH_2ClCF_3$ was obtained. The results from the relative rate study by Green and Wayne (1976) are consistent with the preferred values.

References

Green, R. G. and Wayne, R. P.: *J. Photochem.* 6, 371, 1976.

Warren, R., Gierczak, T. and Ravishankara, A. R.: *Chem. Phys. Lett.*, 183, 403, 1991.