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

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$O(^1D) + CH_2ClCF_3$ (HCFC-133a) $\rightarrow O(^3P) + CH_2ClCF_3$ (1)
$\rightarrow$ other products (2)

$\Delta H°(1) = -190$ kJ mol^{-1}

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

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

Comments

(a) Branching ratio was determined from the ratio of the $O(^3P)$ yield from $O(^1D) + CH_2ClCF_3$ relative to that for $O(^1D) + N_2$.

(b) $O(^1D)$ produced by photolysis of NO_2 at 229 nm. $\Delta(CH_2ClCF_3)/\Delta(N_2O)$ monitored by IR absorption spectroscopy. Measured rate coefficient ratio of $(k_2/k(O(^1D) + N_2O) = 1.3 \pm 0.3$ is placed on an absolute basis using $k(O(^1D) + N_2O) = 1.16 \times 10^{-10}$ cm^3 molecule^{-1} 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 /cm^3 molecule^{-1} s^{-1}	1.2×10^{-10}	298
k_1/k	0.20	298
Reliability		
$\Delta \log k$	± 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 $O(^3P)$ 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.