IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.81 oClOx7

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, https://iupac.pole-ether.fr. This datasheet last evaluated: June 2015; last change in preferred values: November 2003.

$$O(^{1}D) + CHFClCF_{3} (HCFC-124) \rightarrow O(^{3}P) + CHFClCF_{3}$$
 (1)
 \rightarrow other products (2)

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

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

k/cm³ molecule-1 s-1	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients $(8.6 \pm 0.4) \times 10^{-11}$	298	Warren et al., 1991	PLP-RF
Branching Ratios $k_1/k = 0.31 \pm 0.10$	298	Warren et al., 1991	PLP-RF (a)

Comments

(a) Branching ratio was determined from the ratio of the $O(^3P)$ yield from $O(^1D)$ + CHFClCF₃ relative to that for $O(^1D)$ + N_2 .

Preferred Values

Parameter	Value	T/K
k /cm ³ molecule ⁻¹ s ⁻¹	8.6 x 10 ⁻¹¹	298
k_1/k	0.31	298
Reliability		
$\Delta \log k$	± 0.3	298
$\Delta(k_1/k)$	± 0.2	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), the only published study of this reaction. In these experiments, only $O(^3P)$ was monitored and therefore no direct information relating to the products of the chemical reaction of $O(^1D) + CHFCICF_3$ was obtained.

References

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