IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.76 oClOx2

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$O(^1D) + CHFCl_2$(HCFC-21) → ClO + CHFCl (1)
→ other products (2)

$\Delta H°(1) = -113$ 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			
$(1.9 \pm 0.6) \times 10^{-10}$	188-343	Davidson et al., 1978	PLP (a)
Branching Ratios			
$k_1/k = 0.74 \pm 0.15$	298	Takahashi et al., 1996	PLP-LIF (b)
$k_1/k = 0.73 \pm 0.05$	296	Feierabend et al., 2010	PLP-CRDS (c)

Comments

(a) Pulsed laser photolysis of O_3 at 266 nm. $O(^1D)$ atoms were monitored by time-resolved emission at 630 nm.

(b) Branching ratio for ClO formation was determined by measurement of the LIF signal intensity of ClO normalized to that from $O(^1D) + HCl$.

(c) $O(^1D)$ produced by laser photolysis of O_3 at 248 nm. ClO radicals were monitored using cavity ring-down differential absorption spectroscopy near the peak and valley of the 10-0 transition band head at 279.67 and 279.56 nm of the $A^2\pi \leftarrow X^2\pi$ system. Experiments were performed in 400 – 800 mbar of helium diluent.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.9×10^{-10}	180-350
k_1/k	0.74	298
Reliability		
$\Delta \log k$	± 0.3	180-350
$\Delta(k_1/k)$	± 0.1	298

Comments on Preferred Values

The preferred value of k is based on the results of Davidson et al. (1978). The preferred value of

the branching ratio k_1/k is based on the results of Takahashi et al. (1996) and Feierabend et al. (2010).

References

Davidson, J. A., Schiff, H. I., Brown, T. J. and Howard, C. J.: J. Chem. Phys., 69, 4277, 1978.
Feierabend, K.J, Papanastasiou, D.K., and Burkholder, J. B.: J. Phys. Chem. A, 114, 12052, 2010.
Takahashi, K., Wada, R., Matsumi, Y. and Kawasaki, M.: J. Phys. Chem., 100, 10145, 1996.