IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet IV.A2.85 oClOx11

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$$O(^1D) + CCl_4 \rightarrow ClO + CCl_3 \qquad (1)$$
$$\rightarrow O(^3P) + CCl_4 \qquad (2)$$

$\Delta H°(1) = -170$ kJ mol^{-1}
$\Delta H°(2) = -190$ 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			
$(3.1 \pm 0.9) \times 10^{-10}$	203-343	Davidson et al., 1978	PLP (a)
$(3.5 \pm 0.3) \times 10^{-10}$	298	Force and Wiesenfeld, 1981	PLP-RA
Branching Ratios			
$k_2/k = 0.14 \pm 0.06$	298	Force and Wiesenfeld, 1981	PLP-RA (b)
$k_1/k = 0.90 \pm 0.19$	298	Takahashi et al., 1996	PLP-LIF (c)
$k_1/k = 0.79 \pm 0.04$	296	Feierabend et al., 2010	PLP-CRDS (d)

Comments

(a) Pulsed laser photolysis of O_3 at 266 nm. $O(^1D)$ atoms were monitored by time-resolved emission at 630 nm.
(b) $O(^1D)$ atoms were monitored by resonance absorption at 130.4 nm and compared to $O(^3P)$ atoms in the presence of ozone in He diluent where the $O(^3P)$ atom yield from the $O(^1D) + O_3$ reaction is 1.0.
(c) Branching ratio for ClO formation was determined by measurement of the LIF signal intensity of ClO normalized to that from $O(^1D)$ + HCl.
(d) $O(^1D)$ 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}	3.3 x 10^{-10}	200-350
k_1/k	0.79	298
k_2/k	0.21	298
Reliability		
$\Delta \log k$	± 0.1	200-350
$\Delta(k_1/k)$	± 0.1	298
$\Delta(k_2/k)$	± 0.1	298

Preferred Values

k = 3.3 x 10^{-10} cm^3 molecule^{-1} s^{-1} independent of temperature over the range 200-350 K.
k_1/k = 0.79 at 298 K.
k_2/k = 0.21 at 298 K.

Reliability

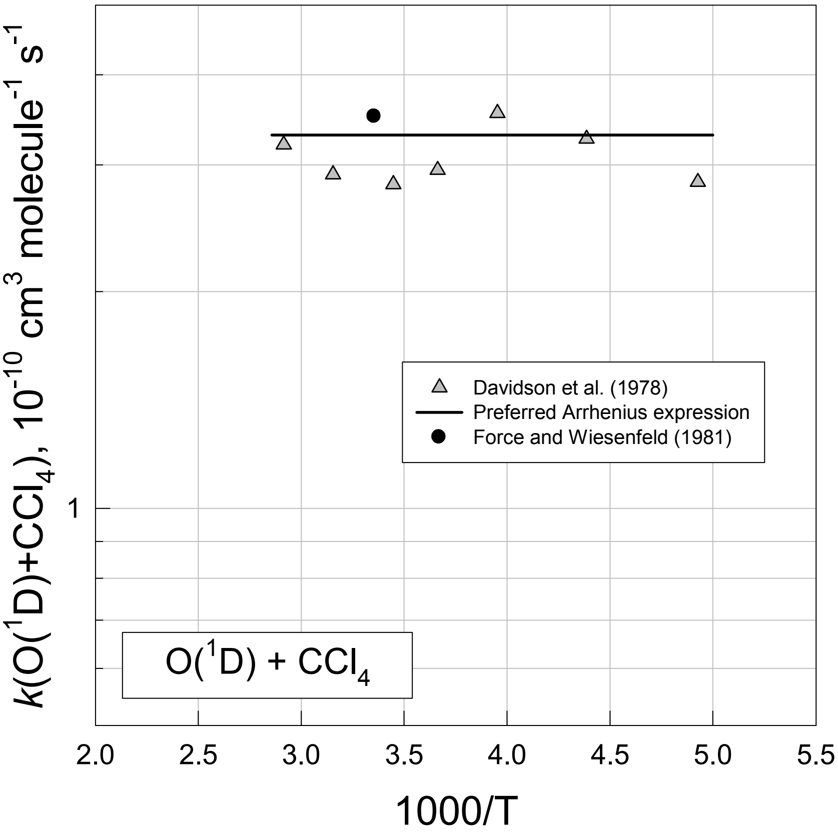
$\Delta \log k$ = ± 0.1 over the temperature range 200-350 K.
$\Delta(k_1/k)$ = ± 0.1 at 298 K.
$\Delta(k_2/k)$ = ± 0.1 at 298 K.

Comments on Preferred Values

The preferred value of k is based on the results of Davidson et al. (1978) and the room temperature result of Force and Wiesenfeld (1981). The preferred value of the branching ratio k_1/k is the value reported by Feierabend et al. (2010) which is consistent with, but more precise than, the measurement by Takahashi et al. (1996). The preferred value of the branching ratio k_2/k is derived from 1 - k_1/k and is consistent with the determination by Force and Wiesenfeld (1981).

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.
Force, A. P., and Wiesenfeld, J. R.: J. Phys. Chem., 85, 782, 1981.
Takahashi, K., Wada, R., Matsumi, Y., and Kawasaki, M.: J. Phys. Chem., 100, 10145, 1996.



k(O(1D)+CCl4), 10-10 cm3 molecule-1 s-1
1
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
1000/T
Davidson et al. (1978)
Preferred Arrhenius expression
Force and Wiesenfeld (1981)
O(1D) + CCl4