IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oRClOx43

This data sheet updated: 27th January 2006.

$CFCl_2O_2 + NO_2 + M \rightarrow CFCl_2O_2NO_2 + M$

$\Delta H° = -107$ kJ mol^{-1}

Low-pressure rate coefficients
Rate coefficient data

k_0/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(3.5 \pm 0.5) \times 10^{-29}$ $[O_2]$	298	Lesclaux and Caralp, 1984	PLP-MS (a)
$(3.5 \pm 0.5) \times 10^{-29}$ $(T/298)^{-4.1}$ $[O_2]$	233-373	Lesclaux, Caralp and Dognon, 1986	PLP-MS (b)
$(5.5 \pm 1.6) \times 10^{-29}$ $(T/298)^{-5.5}$ $[O_2]$	233-373	Caralp et al., 1988	PLP-MS (c)

Comments

(a) Pulsed laser photolysis with MS detection of $CFCl_2O_2$. Pressure range 1.3-13 mbar. Falloff extrapolation with $F_c = 0.6$ and $k_\infty = 6.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}.

(b) As comment (a). Falloff extrapolation with $F_c = 0.6$ and $k_\infty = 5.9 \times 10^{-12}$ $(T/298)^{-0.72}$ cm^3 molecule^{-1} s^{-1}.

(c) As comment (a). Falloff extrapolation using $F_c = \exp(-T/342)$, i. e. $F_c = 0.42$ at 298 K, and $k_\infty = 8.3 \times 10^{-12}$ $(T/298)^{-0.66}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

$k_0 = 5.5 \times 10^{-29}$ $(T/298)^{-5.5}$ $[N_2]$ cm^3 molecule^{-1} s^{-1} over the temperature range 230-380 K.

Reliability

$\Delta \log k_0 = \pm 0.3$ at 298 K.

$\Delta n = \pm 2$.

Comments on Preferred Values

The data from Caralp et al. (1988) are preferred because they employ a value of $F_c = 0.42$. However, this value should be used independent of the temperature. Equal values of k_0 for the bath gases O_2 and N_2 are assumed.

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(6.0 \pm 1.0) \times 10^{-12}$	298	Lesclaux and Caralp, 1984	(a)
$(5.9 \pm 1.0) \times 10^{-12} (T/298)^{-0.72}$	233-373	Lesclaux, Caralp and Dognon, 1986	(b)
$(8.3 \pm 1.0) \times 10^{-12} (T/298)^{-0.66}$	233-373	Caralp et al., 1988	(c)

Comments

(a) See comment (a) for k_0.
(b) See comment (b) for k_0.
(c) See comment (c) for k_0.

Preferred Values

$k_\infty = 8.3 \times 10^{-12} (T/298)^{-0.66}$ cm^3 molecule^{-1} s^{-1} over the temperature range 230-380 K.

Reliability

$\Delta \log k_\infty = \pm 0.2$ at 298 K.
$\Delta n = \pm 0.5$.

Comments on Preferred Values

See Comments on Preferred Values for k_0.

References

Caralp, F., Lesclaux, R., Rayez, M.-T., Rayez, J.-C. and Forst, W.: J. Chem. Soc. Faraday Trans. 2, 84, 569, 1988.
Lesclaux, R. and Caralp, F.: Int. J. Chem. Kinet., 16, 1117, 1984.
Lesclaux, R., Caralp, F. and Dognon, A. M.: Geophys. Res. Lett., 13, 933, 1986.