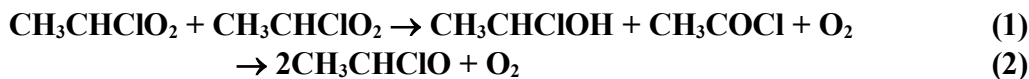


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oRClOx56

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.

This data sheet updated: 27th January 2006.



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

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(5.2 \pm 1.3) \times 10^{-12}$	295	Maricq et al., 1993	(a,b)
<i>Branching Ratios</i>			
$k_2/k = 0.95 \pm 0.05$	295	Maricq et al., 1993	(b)

Comments

- (a) k is defined by $-\text{d}[\text{CH}_3\text{CHClO}_2]/\text{dt} = 2k[\text{CH}_3\text{CHClO}_2]^2$.
- (b) Pulsed photolysis of Cl_2 in the presence of $\text{C}_2\text{H}_5\text{Cl}-\text{O}_2-\text{N}_2$ mixtures with time-resolved IR spectral photography and transient diode laser absorption measurements. The above rate coefficient and branching ratio were obtained from the time-dependence and magnitude of the secondary HCl rise, by computer simulations involving a mechanism of 24 reactions.

Preferred Values

$k_2 = 5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k_2/k = 0.95$ at 298 K.

Reliability

$\Delta \log k_2 = \pm 0.3$ at 298 K.

$\Delta(k_2/k) = \pm 0.05$ at 298 K.

Comments on Preferred Values

While the data of Maricq et al. (1993) for the room temperature rate coefficient seem reasonable in relation to the values of other related halogen-containing peroxy radicals, they have been obtained from very indirect measurements. Confirmation by independent measurements is required to lower the recommended error limits.

References

Maricq, M. M., Shi, J., Szente, J. J., Rimai, L. and Kaiser, E. W.: J. Phys. Chem. 97, 9686, 1993.