IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oRClOx47

This data sheet updated: 27th January 2006.

$$CH_3O_2 + CH_2ClO_2 \rightarrow CH_3O + CH_2ClO + O_2 \quad (1)$$
$$\rightarrow CH_2O + CH_2ClOH + O_2 \quad (2)$$
$$\rightarrow CH_3OH + HC(O)Cl + O_2 \quad (3)$$

Rate coefficient data ($k = k_1 + k_2 + k_3$)

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.5 \pm 0.5) \times 10^{-12}$	298	Villenave and Lesclaux, 1996	PLP-UVA (a)

Comments

(a) Laser flash photolysis of CH_2Cl_2 in the presence of CH_4-O_2-N_2 mixtures at a total pressure of 1013 mbar. Decays in transient absorption signals (with contributions from CH_2ClO_2 and CH_3O_2) were recorded in the wavelength range 220 nm to 250 nm. k derived from simulations of the decay traces using a reaction mechanism which included the self-reactions and reactions with HO_2 of both CH_3O_2 and CH_2ClO_2. A branching ratio of $k_1/k = 0.66$ was assumed for the radical propagating channel, which is the average of the corresponding ratios for the self-reactions of CH_3O_2 and CH_2ClO_2.

Preferred Values

$k = 2.5 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

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

Comments on Preferred Values

The preferred rate coefficient is based on the sole kinetics study of Villenave and Lesclaux (1996). While the value of the rate coefficient appears reasonable, independent verification is required to reduce the recommended error limits.

References

Villenave, E. and Lesclaux, R.: J. Phys. Chem. 100, 14356, 1996.