IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet ROO_30

This data sheet updated: 12th November 2002.

$$CH_3C(O)O_2 + CH_3C(O)CH_2O_2 \rightarrow CH_3C(O)OH + CH_3C(O)CHO + O_2 \quad (1)$$
$$\rightarrow CH_3C(O)O + CH_3C(O)CH_2O + O_2 \quad (2)$$

$\Delta H°(1) = -369$ 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			
$(5.0 \pm 2.0) \times 10^{-12}$	298	Bridier *et al*., 1993[1]	FP-UVAS (a)
$k_1 \leq 4 \times 10^{-12}$	298		
Branching Ratios			
$k_2/k = (0.5 \pm 0.2)$	298	Jenkin *et al*., 1993[2]	P-FTIR-AS (b)

Comments

(a) Flash photolysis of Cl_2 in the presence of $CH_3C(O)CH_3$-CH_3CHO-N_2 mixtures at a total pressure of 1 bar (760 Torr). The rate coefficient k was derived from a kinetic analysis of absorption-time profiles measured at 210 nm, 220 nm, 230 nm and 245 nm, using the value of $k_2/k = 0.5$ determined by Jenkin *et al*.[2]

(b) Steady-state photolysis of Cl_2 in the presence of $CH_3C(O)CH_3$-N_2 mixtures at a total pressure of 930 mbar (700 Torr). The branching ratio was deduced from measurements of the concentrations of the HCHO and $CH_3C(O)CHO$ products by long-path FTIR spectroscopy and long-path UV-VIS diode- array spectroscopy.

Preferred Values

$k = 5.0 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k_2/k = 0.5$ at 298 K.

Reliability

$\Delta \log k = \pm 0.3$ at 298 K.
$\Delta(k_2/k) = \pm 0.2$ at 298 K.

Comments on Preferred Values

The preferred values of the rate coefficient and the branching ratio are from the studies of Bridier *et al*.[1] and Jenkin *et al*.,[2] and require independent confirmation.

References

1 I. Bridier, B. Veyret, R. Lesclaux, and M. E. Jenkin, J. Chem. Soc. Faraday Trans. **89**, 2993 (1993).

2 M. E. Jenkin, R. A. Cox, M. Emrich, and G. K. Moortgat, J. Chem. Soc. Faraday Trans. **89**, 2983 (1993).