IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_20

This data sheet updated: 12th June 2003.

$$\mathbf{2\text{-}C_3H_7O + NO_2 + M \rightarrow \textit{2}\text{-}C_3H_7ONO_2 + M} \quad \mathbf{(1)}$$
$$\mathbf{2\text{-}C_3H_7O + NO_2 \rightarrow CH_3C(O)CH_3 + HONO} \quad \mathbf{(2)}$$

$\Delta H°(1) = -171.7$ kJ·mol^{-1}
$\Delta H°(2) = -277.6$ kJ·mol^{-1}

High-pressure rate coefficients
Rate coefficient data

$k_{\infty 1}$/cm^3 molecule^{-1} s^{-1}	Temp./K	**Reference**	Technique/ Comments
Absolute Rate Coefficients			
3.5×10^{-11}	298	Balla, Nelson and McDonald, 1985[1]	PLP-LIF (a)
$(3.3 \pm 0.3) \times 10^{-11}$	296	Mund, Fockenberg and Zellner, 1998[2]	PLP-LIF (b)

Comments

(a) By extrapolation to zero laser power, a rate coefficient of $k_{\rightarrow 1} = 1.5 \times 10^{-11} \exp[(250 \pm 200)/T]$ cm^3 molecule^{-1} s^{-1} was derived from measurements over the temperature range 295 K to 384 K. No pressure dependence was observed between 1.3 mbar and 13 mbar.

(b) The measured rate coefficient was observed to be independent of total pressure over the range 6.7 mbar to 106 mbar of He.

Preferred Values

$k_{\infty 1} = 3.4 \times 10^{-11}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 200-300 K.

Reliability

$\Delta \log k_{\infty 1} = \pm 0.2$ at 298 K.

Comments on Preferred Values

The recommendation is based on the data of Balla *et al.*[1] and Mund *et al.*[2] The value of $k_{\infty 1}$ is consistent with other related reactions such as RO + NO + M → RONO + M and RO + NO_2 + M → $RONO_2$ + M (with R = CH_3, C_2H_5, *i*-C_3H_7, see this evaluation). It is estimated that $k_2/k_{\rightarrow 1}$ <0.2 (Suppl. IV). Batt[3] cites a rate coefficient ratio of $k_2/k_1 = 0.027 \pm 0.006$ at ~450 K, indicating that reaction (2) is of negligible importance under atmospheric conditions.

References

1 R. J. Balla, H. H. Nelson, and J. R. McDonald, Chem. Phys. **99**, 323 (1985).
2 Ch. Mund, Ch. Fockenberg, and R. Zellner, Ber. Bunsenges. Phys. Chem. **102**, 709 (1998).
3 L. Batt, Int. Rev. Phys. Chem. **6**, 53 (1987).