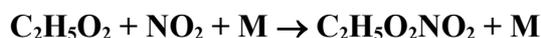


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A6.130 ROO_11

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$$\Delta H^\circ = -67.7 \text{ kJ}\cdot\text{mol}^{-1}$$

Low-pressure rate coefficients Rate coefficient data

$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i> $4.8 \times 10^{-29} [\text{N}_2]$	254	Elfers, Zabel, and Becker, 1990 ¹	(a)

Comments

- (a) Thermal decomposition of $\text{C}_2\text{H}_5\text{O}_2\text{NO}_2$ in a glass reaction chamber in the presence of differing initial $[\text{NO}_2]/[\text{NO}]$ ratios at total pressures of 10 mbar to 1000 mbar. $\text{C}_2\text{H}_5\text{O}_2\text{NO}_2$ was prepared *in situ* by the photolysis of $\text{Cl}_2\text{-C}_2\text{H}_6\text{-O}_2\text{-NO}_2\text{-N}_2$ mixtures. $\text{C}_2\text{H}_5\text{O}_2\text{NO}_2$, NO_2 and NO concentrations were monitored by longpath FTIR absorption and rate coefficient ratios for the reaction of $\text{C}_2\text{H}_5\text{O}_2$ with NO and NO_2 were obtained. The reported rate coefficient for $\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_2$ was derived using a rate coefficient of $8.9 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction $\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{C}_2\text{H}_5\text{O} + \text{NO}_2$. Falloff curves were constructed based on the theoretical analysis from ref. 2 with $F_c = 0.31$ and $k_\infty = 7.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

Preferred Values

$$k_0 = 1.3 \times 10^{-29} (T/300)^{-6.2} [\text{N}_2] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the temperature range 200 K to 300 K.}$$

Reliability

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

$$\Delta n = \pm 1.$$

Comments on Preferred Values

The preferred values are based on the data from ref. 1 and the analysis from ref. 2. The temperature dependence is from the theoretical analysis of ref. 2. Falloff extrapolations were made with $F_c = 0.31$ at 250 K to 300 K such as given from the theoretical analysis of ref. 2.

High-pressure rate coefficients Rate coefficient data

$k_{\infty}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i> 1.0×10^{-11}	254	Elfers, Zabel, and Becker, 1990 ¹	(a)

Comments

(a) See comment (a) for k_0 .

Preferred Values

$k = 5.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K and 1 bar of air.

$k_{\infty} = 8.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, independent of temperature over the range 200 K to 300 K.

Reliability

$\Delta \log k_{\infty} = \pm 0.3$ over the temperature range 200 K to 300 K.

Comments on Preferred Values

See comments on k_0 . The theoretical analysis in ref. 2 also includes information from studies of the reverse reaction measured in ref. 3.

The following text-line combines the preferred values for the high and low pressure limiting rate coefficients to generate a single, cut-and-paste expression for calculation of k :

$$= ((1.3e-29*(T/300)^{-6.2}*M*(8.8e-12))/((1.3e-29*(T/300)^{-6.2}*M+(8.8e-12))*10^{(\log10(0.31)/(1+(\log10((1.3e-29*(T/300)^{-6.2}*M/(8.8e-12))/(0.75-1.27*\log10(0.31))))^2}))$$

The molecular density, $M = 7.243 \times 10^{21} P(\text{bar})/T(\text{K})$

References

- ¹ G. Elfers, F. Zabel, and K. H. Becker, Chem. Phys. Lett. **168**, 14 (1990).
- ² M. Destriau and J. Troe, Int. J. Chem. Kinet. **22**, 915 (1990).
- ³ F. Zabel, A. Reimer, K. H. Becker, and E. H. Fink, J. Phys. Chem. **93**, 5500 (1989).