

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A5.113 RO_14

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$$\Delta H^\circ(2) = -142.2 \text{ kJ mol}^{-1}$$

High-pressure rate coefficients Rate coefficient data

$k_{\infty 1}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
3.4×10^{-11}	298	Balla, Nelson, and McDonald, 1985 ¹	PLP-LIF (a)
$(3.3 \pm 0.1) \times 10^{-11} (T/300)^{-1.3}$	286-389	Fittschen <i>et al.</i> , 1999 ²	PLP-LIF (b)

Comments

- (a) No pressure dependence of the rate coefficient was observed over the range 1.3-6 mbar. The small negative temperature dependence [$k = 1.2 \times 10^{-11} \exp(310/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$] observed over the range 298-383 K may be attributed to falloff effects.
- (b) Measurements over the range 39-658 mbar of He. Results assumed to be in the high pressure range. The observed T-dependence corresponding to $k_{\infty 1} = 8.9 \times 10^{-12} \exp(+397/K)$ maybe attributed to falloff effects.

Preferred Values

$$k_{\infty 1} = 3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_2 = 6.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K and } 27\text{-}270 \text{ mbar pressure.}$$

Reliability

$$\Delta \log k_{\infty 1} = \pm 0.3 \text{ at } 298 \text{ K.}$$

$$\Delta \log k_2 = \pm 0.5 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred value of $k_{\infty 1}$ is based on the study of Balla *et al.*¹ and Fittschen *et al.*². The apparent temperature coefficient of $k_{\infty 1}$ differs from that of $k_{\infty 1}$ for $\text{C}_2\text{H}_5\text{O} + \text{NO} + \text{M}$. It remains to be clarified whether falloff effects are responsible for the different behavior. The value of k_2 is obtained from the preferred $k_{\infty 1}$ and the rate coefficient ratio $k_2/k_1 = 0.19 \pm 0.03$ (independent of temperature) cited in Ref. 3.

References

- ¹ R. J. Balla, H. H. Nelson, and J. R. McDonald, *Chem Phys.* **99**, 323 (1985).
- ² C. Fittschen, A. Frenzel, K. Imrik, and P. Devolder, *Int. J. Chem. Kinet.* **31**, 800 (1999).
- ³ L. Batt and R. T. Milne, *Int. J. Chem. Kinet.* **9**, 141 (1977).