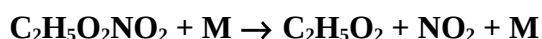


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A6.131 ROO\_12

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This datasheet last evaluated: June 2009. Last change in preferred values: June 2003.



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

### Low-pressure rate coefficients Rate coefficient data

$k_0/\text{s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$4.8 \times 10^{-4} \exp(-9285/T) [\text{N}_2]$	245-273	Zabel <i>et al.</i> , 1989 <sup>1</sup>	FTIR (a)

### Comments

- (a) Unimolecular decay of  $\text{C}_2\text{H}_5\text{O}_2\text{NO}_2$  followed at total pressures ranging from 10 mbar to 800 mbar. Falloff extrapolation with  $F_c = 0.3$ .

### Preferred Values

$$k_0 = 1.4 \times 10^{-17} [\text{N}_2] \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

$$k_0 = 4.8 \times 10^{-4} \exp(-9285/T) [\text{N}_2] \text{ s}^{-1} \text{ over the temperature range } 250 \text{ K to } 300 \text{ K.}$$

### Reliability

$$\Delta \log k_0 = \pm 0.5 \text{ at } 298 \text{ K.}$$

$$\Delta (E/R) = \pm 1000 \text{ K.}$$

### Comments on Preferred Values

The dissociation data are consistent with experimental recombination data from ref. 2 and the theoretical analysis from refs. 1 and 3. Falloff curves are constructed with  $F_c = 0.31$  (over the range 250 K to 300 K).

### High-pressure rate coefficients Rate coefficient data

$k_\infty/\text{s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			

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$8.8 \times 10^{15} \exp(-10440/T)$

245-273

Zabel *et al.*, 1989<sup>1</sup>

FTIR (a)

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### Comments

(a) See comment (a) for  $k_0$ .

### Preferred Values

$k = 3.4 \text{ s}^{-1}$  at 298 K and 1 bar of air.

$k_\infty = 5.4 \text{ s}^{-1}$  at 298 K.

$k_\infty = 8.8 \times 10^{15} \exp(-10440/T) \text{ s}^{-1}$ , over the temperature range 250 K to 300 K.

### Reliability

$\Delta \log k_\infty = \pm 0.5$  at 300 K.

$\Delta(E/R) = \pm 1000 \text{ K}$ .

### Comments on Preferred Values

See comments on  $k_0$ .

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  $k$ :

$$= ((4.8e-4 * \exp(-9285/T)) * M * (8.8e15 * \exp(-10440/T))) / ((4.8e-4 * \exp(-9285/T)) * M + (8.8e15 * \exp(-10440/T)) * 10^{(\log_{10}(0.31) / (1 + (\log_{10}((4.8e-4 * \exp(-9285/T)) * M / (8.8e15 * \exp(-10440/T))) / (0.75 - 1.27 * \log_{10}(0.31))))^2})$$

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

### References

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