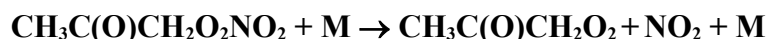


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet ROO_17

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This data sheet updated: 19th December 2005.



High-pressure rate coefficients Rate coefficient data

k_∞/s^{-1}	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$1.9 \times 10^{16} \exp(-10830/T)$	250-298	Sehested <i>et al.</i> , 1998	(a)
~ 3	295		
$1.0 \times 10^{16} \exp(-10630/T)$	246-262	Kirchner <i>et al.</i> , 1999	(a)

Comments

- (a) Loss of $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2\text{NO}_2$, which was produced by static photolysis in a 140 l pyrex reaction chamber at pressure of 933 mbar, was followed by long path FTIR. k at room temperature (295 K) obtained by fitting acetyl peroxy nitrate decay with a complex mechanism. Data for low temperature (250-275 K) were obtained directly from the decay of preformed $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2\text{NO}_2$ after the addition of excess NO.
- (b) Experiments in a 420 l reaction chamber with photolytic generation of radicals forming peroxy nitrates. Decomposition of acetyl peroxy nitrate in the dark followed by FTIR spectrometry. Measurements in 10, 100, and 800 mbar of N_2 . Rate coefficients at 10 mbar are about a factor of 2 smaller than at 800 mbar.

Preferred Values

$k_\infty = 1.4 \times 10^{16} \exp(-10730/T) \text{ s}^{-1}$ over the temperature range 240 to 260 K.

Reliability

$\Delta \log k_\infty = \pm 0.3$ at 250 K.

$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The results from the two experimental studies are essentially in agreement, and are consistent with data for related reactions. The preferred Arrhenius parameters are a simple mean of the reported experimental values. The measured rate coefficients are expected, by analogy with the corresponding PAN decomposition at 1 bar of air (IUPAC, 2002), to be very close to the high pressure limit.

References

IUPAC, <http://iupac.pole-ether.fr>, 2013.

Kirchner, F., Mayer-Figge, A., Zabel, F. and Becker, K. H., *Int. J. Chem. Kinet.* 31, 127, 1999.

Sehested, J., Christenson, L. K., Nielsen, O. J., Bilde, M., Wallington, T. J., Schneider, W. F., Orlando, J. J. and Tyndall, G. S., *Int. J. Chem. Kinet.* 30, 475, 1998.