IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC12

Website: http://iupac.pole-ether.fr. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

This data sheet updated: 18th October 2007 (with revision of the preferred values).

$NO_3 + CH_3CH_2CHO \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.7 \times 10^{-11} \exp[-(2250 \pm 192)/T]$	298-433	Cabañas et al., 2001	DF-LIF
$(6.0 \pm 0.6) \times 10^{-15}$	298 ± 2		
$(5.8 \pm 1.0) \times 10^{-15}$	300 ± 3	Bossmeyer et al., 2006	DOAS/GC (a)
Relative Rate Coefficients			
$(5.80 \pm 0.48) \times 10^{-15}$	298 ± 2	D'Anna and Nielsen, 1997	RR (b)
$(7.28 \pm 0.41) \times 10^{-15}$	296 ± 2	Papagni et al., 2001	RR (c)
$(6.18 \pm 0.57) \times 10^{-15}$	298 ± 2	D'Anna et al., 2001	RR (b)

Comments

(a) Carried out in the EUPHORE chamber at atmospheric pressure of air. NO_3 radical concentrations measured by DOAS, and propanal concentrations by GC.

(b) NO_3 radicals were generated by the thermal dissociation of N_2O_5. Experiments were carried out in 1 atmosphere of air with measurements of propanal and propene (the reference compound) by FTIR spectroscopy. The measured rate coefficient ratios $k(NO_3 + \text{propanal})/k(NO_3 + \text{propene}) = 0.61 \pm 0.05$ (D'Anna and Nielsen, 1997) and 0.65 ± 0.06 (D'Anna et al., 2001) are placed on an absolute basis by use of a rate coefficient of $k(NO_3 + \text{propene}) = 9.5 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K (IUPAC, current recommendation).

(c) NO_3 radicals were generated by the thermal dissociation of N_2O_5. Experiments were carried out in 1 atmosphere of air with measurements of propanal and methacrolein (the reference compound) by GC. The measured rate coefficient ratio $k(NO_3 + \text{propanal})/k(NO_3 + \text{methacrolein}) = 2.14 \pm 0.12$ is placed on an absolute basis by use of a rate coefficient of $k(NO_3 + \text{methacrolein}) = 3.4 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 296 K (IUPAC, current recommendation).

Preferred Values

$k = 6.3 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.15$ at 298 K.

Comments on Preferred Values

The preferred 298 K rate coefficient is the average of the room temperature absolute rate coefficient of Bossmeyer et al. (2006) and the relative rate coefficients of D'Anna and Nielsen (1997), D'Anna et al. (2001) and Papagni et al. (2001), which are in reasonable agreement and which also agree with the measured absolute room temperature rate coefficient of Cabañas et al. (2001). Because of the higher temperature dependence obtained by Cabañas et al. (2001) for the reactions of NO_3 radicals with acetaldehyde and butanal than by other investigators (see data sheets) and because the rate coefficient at 298 K calculated from the Arrhenius expression of Cabañas et al. (2001) is 50% higher than their measured value, the Cabañas et al. (2001) data are not used in the evaluation of the rate coefficient for this reaction. No recommendation is made concerning the temperature dependence for this reaction.

References

Bossmeyer, J., Brauers, T., Richter, C., Rohrer, F., Wegener, R. and Wahner, A.: Geophys. Res. Lett. 33, L18810, doi: 10.1029/2006GL026778, 2006.

Cabañas, B., Martín, P., Salgado, S., Ballesteros, B. and Martínez, E.: J. Atmos. Chem. 40, 23, 2001.

D'Anna, B. and Nielsen, C. J.: J. Chem. Soc. Faraday Trans. 93, 3479, 1997.

D'Anna, B., Andresen, Ø., Gefen, Z. and Nielsen, C. J.: Phys. Chem. Chem. Phys. 3, 3057, 2001.

IUPAC, http://iupac.pole-ether.fr, 2007.

Papagni, C., Arey, J. and Atkinson, R.: Int. J. Chem. Kinet. 32, 79, 2001.