IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC2

This data sheet updated: 29th October 2007 (with no revisions of the preferred values).

$NO_3 + C_2H_2 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$4.9 \times 10^{-13} \exp[-(2742 \pm 542)/T]$	295-523	Canosa-Mas et al., 1988a,b	DF-A
$(5.1 \pm 3.5) \times 10^{-17}$	295 ± 2		
Relative Rate Coefficients			
$\leq 3.0 \times 10^{-17}$	298 ± 2	Atkinson et al., 1987	RR (a)

Comments

(a) NO_3 radicals were generated by the thermal decomposition of N_2O_5. The concentrations of acetylene and ethene (the reference organic) were measured by GC. The measured rate coefficient ratio of $k(NO_3 + C_2H_2)/k(NO_3 + C_2H_4) \leq 0.14$ at 298 ± 2 K is placed on an absolute basis by use of a rate coefficient of $k(NO_3 + C_2H_4) = 2.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

Preferred Values

$k < 1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

The measurement of rate coefficients for low reactivity organics is complicated by the possibility of secondary reactions, leading to erroneously high measured rate coefficients. The relative rate measurements of Atkinson et al. (1987) show C_2H_2 to be significantly less reactive than C_2H_4. The preferred value of the upper limit to the rate coefficient is sufficiently high to be consistent with the data of Canosa-Mas et al. (1988a). Until there are confirmatory data for the reported temperature dependence (Canosa-Mas et al., 1988b) of this rate coefficient, no temperature dependence is recommended.

References

Atkinson, R., Aschmann, S. M. and Goodman, M. A.: Int. J. Chem. Kinet., 19, 299, 1987.

Canosa-Mas, C., Smith, S. J., Toby, S. and Wayne, R. P.: J. Chem. Soc. Faraday Trans. 2, 84, 247, 1988a.

Canosa-Mas, C., Smith, S. J., Toby, S. and Wayne, R. P.: J. Chem. Soc. Faraday Trans. 2, 84, 263, 1988b.

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