IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx81

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$NO_3 + C_2Cl_4 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(9.6 \pm 8.1) \times 10^{-17}$	295	Noremsaune et al., 1997	DF-Vis (a)
Relative Rate Coefficients			
$<5 \times 10^{-17}$	298	Atkinson et al., 1987	RR (b)
$(8 \pm 3) \times 10^{-17}$	299	Noremsaune et al., 1997	RR (c)
4×10^{-17}	299	Noremsaune et al., 1997	RR (d)
$<1.8 \times 10^{-16}$	298	Chew et al., 1998	RR (e)

Comments

(a) NO_3 generated by F + HNO_3 and detected by optical absorption in a multi-pass cell. Experiments conducted under pseudo-first order conditions.

(b) Derived by monitoring the relative decay rates of C_2Cl_4 and C_2H_4 in N_2O_5-NO_2-organic-air mixtures at one atmosphere total pressure of air. The observations yielded $k(NO_3 + C_2Cl_4)/k(NO_3 + C_2H_4) = < 0.25$. This upper limit to the rate coefficient ratio was placed on an absolute basis by use of $k(NO_3 + C_2H_4) = 2.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

(c) NO_3 formed in the thermal decomposition of N_2O_5 in mixtures containing C_2HCl_3 and ethene as reference reactant at total pressures of 1013 mbar N_2. Addition of ethane as Cl atom scavenger had no effect. $k(NO_3 + C_2Cl_4)/k(NO_3 + C_2H_4)$ was measured to be (0.39 ± 0.11). This was placed on an absolute basis using $k(NO_3 + C_2H_4) = 2.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

(d) NO_3 formed in the thermal decomposition of N_2O_5 in mixtures containing C_2Cl_4 and C_2H_3Cl as reference reactant at total pressures of 1013 mbar N_2. Addition of ethane as Cl atom scavenger had no effect. $k(NO_3 + C_2Cl_4)/k(NO_3 + C_2H_3Cl)$ was measured to be 0.1. This was placed on an absolute basis using $k(NO_3 + C_2H_3Cl) = (3.7 \pm 0.8) \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Noremsaune et al. 1997).

(e) NO_3 formed in the thermal decomposition of N_2O_5 in mixtures containing C_2Cl_4 and 2,3-dimethylbutane as reference reactant at total pressures of 990 mbar air. Depletion of reactants was monitored by GC-FID. Addition of ethane as Cl and OH atom scavenger. $k(NO_3 + C_2Cl_4)/k(NO_3 + 2,3\text{-dimethylbutane})$ was measured to be (0.21 ± 0.18). This was placed on an absolute basis using $k(NO_3 + 2,3\text{-dimethylbutane}) = 4.39 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

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

Comments on Preferred Values

The preferred value is derived from the relative rate coefficients measured by Atkinson et al. (1987). The upper limit to the rate coefficient has been increased in order to take into account the spread in the data.

References

Atkinson, R. A., Aschmann, S. M., and Goodman, M. A.: Int. J. Chem. Kinet., 19, 299, 1987.
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Noremsaune, I. M. W., Langer, S., Ljungström, E. and Nielsen, C. J.: J. Chem. Soc., Faraday Trans. 93, 525, 1997.
Perez-Casany, M. P., Nebot-Gil, I. and Sanchez-Martin, J.: J. Phys. Chem. A,. 104, 11340, 2000.