Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC44

The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, (http://iupac.pole-ether.fr)
This datasheet last evaluated: June 2015; last change in preferred values: June 2015.

$NO_3 + (HCO)_2 \rightarrow HC(O)CO + HNO_3$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(4.2 \pm 0.8) \times 10^{-16}$	296	Talukdar et al., 2011	FT-CIMS (a)
$(7.9 \pm 3.6) \times 10^{-16}$	353		
Relative Rate Coefficients			
$(4.0 \pm 1.0) \times 10^{-16}$	296	Talukdar et al., 2011	RR (b)
$(3.4 \pm 0.2) \times 10^{-16}$			RR (c)

Comments

(a) Flow tube operated at 2-6 Torr He. NO_3 (initially 1-5 $\times$ 10^{11} molecule cm^{-3}) was generated from the thermal decomposition of N_2O_5 and detected with iodide-CIMS. $(HCO)_2$ was in 1000 fold excess over NO_3.

(b) Experiments in 22 L Pyrex reactor at 840 mbar air. NO_3 was generated by the thermal decomposition of N_2O_5, $(HCO)_2$ and the reference reactant (C_2H_4) were monitored ex-situ using FTIR. $CF_3CF{=}CHF$ was added as OH scavenger. The rate coefficient ratio, $k(NO_3 + (HCO)_2) / k(NO_3 + C_2H_4) = 1.9 \pm 0.2$, 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).

(c) As (b) but with or $(CH_3)_2CH_2CH_3$) as reference reactant. The rate coefficient ratio, $k(NO_3 + (HCO)_2) / k(NO_3 + (CH_3)_2CH_2CH_3) = 3.1 \pm 0.2$, was placed on an absolute basis using $k(NO_3 + (CH_3)_2CH_2CH_3) = 1.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	4×10^{-16}	290 – 350 K

Reliability

$\Delta \log k$	± 0.15	298

Comments on Preferred Values

The studies of the reaction between NO_3 and glyoxal, $(HCO)_2$, were measured by the same group (Talukdar et al., 2011), who obtained satisfactory agreement between absolute and relative methods covering a large range of pressures. The authors suggest that the error associated with the absolute measurement of this slow reaction at 296 and 353 K are too large to warrant determination of the temperature dependence. We therefore prefer a temperature independent value of 4×10^{-16} cm^3 $molecule^{-1}$ s^{-1} with extended error limits. The reaction products were not determined, but the authors argue that H-abstraction will dominate.

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References

IUPAC, Task group on atmospheric chemical kinetic data evaluation. (Ammann, M., Atkinson, R., Cox, R.A., Crowley, J.N., Herrmann, H., Jenkin, M.E., Mellouki, W., Rossi, M. J., Troe, J. and Wallington, T. J.) http://iupac.pole-ether.fr, 2015.

Talukdar, R. K., Zhu, L., Feierabend, K. J., and Burkholder,J. B.: Atmos. Chem. Phys. 11, 10837-10851, 2011.