Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC45

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.

$NO_3 + CH_3C(O)CHO \rightarrow CH_3C(O)CO + HNO_3$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(5.0 \pm 2.1) \times 10^{-16}$	296	Talukdar et al., 2011	RR (a)

Comments

(a) Experiments in a 22 L Pyrex reactor at 840 mbar air. NO_3 was generated by the thermal decomposition of N_2O_5. $CH_3C(O)CHO$ 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, $k(NO_3 + CH_3C(O)CHO) / k(NO_3 + C_2H_4)$, was measured with two different $CH_3C(O)CHO$ samples to give values of 2.9 ± 0.5 and 1.9 ± 0.2. We combine the average result (2.4 ± 1.0) with $k(NO_3 + C_2H_4) = 2.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation) to derive the value listed in the table.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	5×10^{-16}	298 K
Reliability		
$\Delta \log k$	± 0.3	298

Comments on Preferred Values

The single and limited rate coefficient determination (Talukdar et al., 2011) of the reaction between NO_3 and $CH_3C(O)CHO$ (methylglyoxal) suffered from poor reproducibility and carries significant uncertainty. We prefer a value of $k = 5 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} and extend the uncertainty reported by Talukdar et al. 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.