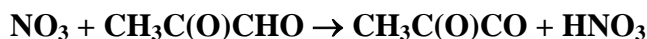


## Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO<sub>3</sub>\_VOC45

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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.



### Rate coefficient data

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

### Comments

- (a) Experiments in a 22 L Pyrex reactor at 840 mbar air. NO<sub>3</sub> was generated by the thermal decomposition of N<sub>2</sub>O<sub>5</sub>. CH<sub>3</sub>C(O)CHO and the reference reactant (C<sub>2</sub>H<sub>4</sub>) were monitored ex-situ using FTIR. CF<sub>3</sub>CF=CHF was added as OH scavenger. The rate coefficient ratio,  $k(\text{NO}_3 + \text{CH}_3\text{C}(\text{O})\text{CHO}) / k(\text{NO}_3 + \text{C}_2\text{H}_4)$ , was measured with two different CH<sub>3</sub>C(O)CHO samples to give values of  $2.9 \pm 0.5$  and  $1.9 \pm 0.2$ . We combine the average result ( $2.4 \pm 1.0$ ) with  $k(\text{NO}_3 + \text{C}_2\text{H}_4) = 2.1 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  (IUPAC, current recommendation) to derive the value listed in the table.

### Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$5 \times 10^{-16}$	298 K
<i>Reliability</i> $\Delta \log k$	$\pm 0.3$	298

### Comments on Preferred Values

The single and limited rate coefficient determination (Talukdar et al., 2011) of the reaction between NO<sub>3</sub> and CH<sub>3</sub>C(O)CHO (methylglyoxal) suffered from poor reproducibility and carries significant uncertainty. We prefer a value of  $k = 5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  and extend the uncertainty reported by Talukdar et al. The reaction products were not determined, but the authors argue that H-abstraction will dominate.

## 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.