# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO3_VOC3

Website: http://iupac.pole-ether.fr. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission.

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

---

## $NO_3 + C_2H_4 \rightarrow$ products

### Rate coefficient data

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/ Comments |
|---|---|---|---|
| *Absolute Rate Coefficients* | | | |
| $6.29 \times 10^{-12} \exp[-(3103 \pm 145)/T]$ | 295-523 | Canosa-Mas et al., 1988a,b | DF-A |
| $(1.85 \pm 0.24) \times 10^{-16}$ | $295 \pm 2$ | | |
| $(1.7 \pm 0.5) \times 10^{-16}$ | 300 | Biggs et al., 1991; Boyd et al., 1991 | (a) |
| *Relative Rate Coefficients* | | | |
| $(2.16 \pm 0.20) \times 10^{-16}$ | $296 \pm 2$ | Atkinson et al., 1988 | RR (b) |

### Comments

(a) Stopped-flow technique with optical absorption of the $NO_3$ radical at 662 nm. The influence of the reaction $NO_2 + NO_3 + He \rightarrow N_2O_5 + He$ was taken into account by numerical modeling, leading to a stoichiometry factor for $NO_3$ radical decays of ~1.9 and the cited rate coefficient for the elementary $NO_3$ + ethene reaction.

(b) $NO_3$ radicals were generated by the thermal decomposition of $N_2O_5$. A series of rate coefficient ratios were measured, with the concentrations of the organic compounds involved being measured by GC. Based on rate coefficient ratios for the sets of organic compounds ethene *vs*. 2,3-dimethylbutane, 2,3-dimethylbutane *vs*. tetrahydrofuran, tetrahydrofuran *vs*. propene, propene *vs*. thiophene, thiophene *vs*. bicyclo[2.2.2]-2-octene, and bicyclo[2.2.2]-2-octene *vs*. *trans*-2-butene, a rate coefficient ratio of $k(NO_3 + \text{ethene})/k(NO_3 + \textit{trans}\text{-2-butene}) = 0.000554 \pm 0.000050$ was obtained. This rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of $k(NO_3 + \textit{trans}\text{-2-butene}) = 3.89 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 296 K (Atkinson, 1997).

### Preferred Values

$k = 2.1 \times 10^{-16}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K.

$k = 3.3 \times 10^{-12} \exp(-2880/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ over the temperature range 270-340 K.

*Reliability*

$\Delta \log k = \pm 0.2$ at 298 K.

$\Delta(E/R) = \pm 500$ K.

*Comments on Preferred Values*

The preferred rate coefficient is derived using the absolute rate coefficient data of Canosa-Mas et al. (1988a,b) and the relative rate coefficient of Atkinson et al. (1988). These data were fitted to the three parameter expression $k = CT^2 \exp(-D/T)$, resulting in $k = 4.88 \times 10^{-18} T^2 \exp(-2282/T)$ cm$^3$ molecule$^{-1}$ s$^{-1}$ over the temperature range 295-523 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 300 K and is derived from the three parameter expression with $A = C e^2 T^2$ and $B = D + 2T$.

The preferred rate coefficient is in agreement with the 300 K rate coefficient of Biggs et al. (1991) and Boyd et al. (1991).

## References


Atkinson, R.: J. Phys. Chem. Ref. Data, 26, 215, 1997.

Atkinson, R., Aschmann, S. M. and Pitts Jr., J. N.: J. Phys. Chem., 92, 3454, 1988.

Biggs, P., Boyd, A. A., Canosa-Mas, C. E., Joseph, D. M. and Wayne, R. P.: Meas. Sci. Technol., 2, 675, 1991.

Boyd, A. A., Canosa-Mas, C. E., King, A. D., Wayne, R. P. and Wilson, M. R.: J. Chem. Soc. Faraday Trans., 87, 2913, 1991.

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.