

# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO<sub>3</sub>\_AROM1

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## NO<sub>3</sub> + C<sub>6</sub>H<sub>6</sub> (Benzene) → products

### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$\leq 5 \times 10^{-17}$	300	Japar and Niki, 1975	RR (a)
$\leq 2.7 \times 10^{-17}$	298 ± 1	Atkinson et al., 1984a	RR (b)
$< 6 \times 10^{-17}$	298 ± 1	Atkinson et al., 1984b	RR (c)

### Comments

- (a) NO<sub>3</sub> radicals were generated from the thermal decomposition of N<sub>2</sub>O<sub>5</sub>. The experimental data were relative to the equilibrium coefficient  $K$  for the NO<sub>3</sub> + NO<sub>2</sub> ↔ N<sub>2</sub>O<sub>5</sub> reactions, and are placed on an absolute basis by use of  $K = 2.15 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1}$  at 300 K (IUPAC, current recommendation).
- (b) NO<sub>3</sub> radicals were generated from the thermal decomposition of N<sub>2</sub>O<sub>5</sub>. The concentrations of benzene and ethene (the reference compound) were measured by GC, and a rate coefficient ratio of  $k(\text{NO}_3 + \text{benzene})/k(\text{NO}_3 + \text{ethene}) \leq 0.13$  obtained. This rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of  $k(\text{NO}_3 + \text{ethene}) = 2.1 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (IUPAC, current recommendation).
- (c) NO<sub>3</sub> radicals were generated from the thermal decomposition of N<sub>2</sub>O<sub>5</sub>. The concentrations of toluene and *n*-heptane (the reference compound) were measured by GC. The measured rate coefficient ratio of  $k(\text{NO}_3 + \text{benzene})/k(\text{NO}_3 + \textit{n}\text{-heptane}) < 0.4$  is placed on an absolute basis by use of a rate coefficient of  $k(\text{NO}_3 + \textit{n}\text{-heptane}) = 1.5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K (Atkinson and Arey, 2003).

### Preferred Values

$k < 3 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

#### Comments on Preferred Values

All three room temperature relative rate measurements (Japar and Niki, 1975; Atkinson et al., 1984a,b) obtained only upper limits to the rate coefficient. These studies are the basis for the preferred value.

## References

Atkinson, R. and Arey, J.: Chem. Rev., 103, 4605, 2003.

Atkinson, R., Plum, C. N., Carter, W. P. L., Winer, A. M. and Pitts Jr., J. N.: J. Phys. Chem., 88, 1210, 1984a.

Atkinson, R., Carter, W. P. L., Plum, C. N., Winer, A. M. and Pitts Jr., J. N.: Int. J. Chem. Kinet., 16, 887, 1984b.

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Japar, S. M. and Niki, H.: J. Phys. Chem., 79, 1629, 1975.