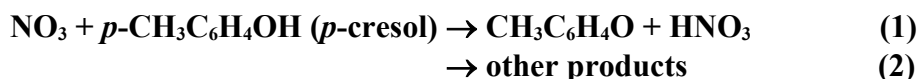


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet NO₃_AROM5

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 last evaluated September 2008; last change in preferred values September 2008.



Rate coefficient data ($k = k_1 + k_2$)

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(1.50 \pm 0.24) \times 10^{-11}$	300 ± 1	Carter et al., 1981	RR (a)
$(1.38 \pm 0.15) \times 10^{-11}$	298 ± 1	Atkinson et al., 1984	RR (b)
$(1.07 \pm 0.10) \times 10^{-11}$	296 ± 2	Atkinson et al., 1992	RR (c)

Comments

- (a) NO₃ radicals were generated from the reaction of O₃ with NO₂ in the presence of *p*-cresol and 2-methyl-2-butene (the reference compound) at atmospheric pressure of air. The contribution of the O₃ reaction was taken into account in estimating the amount of 2-methyl-2-butene reacted with NO₃ radicals. The concentrations of *p*-cresol and 2-methyl-2-butene were monitored by GC. The derived rate coefficient ratio is placed on an absolute basis using a rate coefficient of $k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).
- (b) NO₃ radicals were generated from the thermal decomposition of N₂O₅ in the presence of *p*-cresol and *m*-cresol (the reference compound) at atmospheric pressure of air. The concentrations of *p*- and *m*-cresol were monitored by GC. The measured rate coefficient ratio of $k(\text{NO}_3 + p\text{-cresol})/k(\text{NO}_3 + m\text{-cresol}) = 1.38 \pm 0.15$ is placed on an absolute basis using a rate coefficient of $k(\text{NO}_3 + m\text{-cresol}) = 1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation).
- (c) NO₃ radicals were generated from the thermal decomposition of N₂O₅ in the presence of *p*-cresol and 2-methyl-2-butene (the reference compound) at atmospheric pressure of air. The concentrations of *p*-cresol and 2-methyl-2-butene were monitored by GC. The measured rate coefficient ratio of $k(\text{NO}_3 + p\text{-cresol})/k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 1.14 \pm 0.10$ is placed on an absolute basis using a rate coefficient of $k(\text{NO}_3 + 2\text{-methyl-2-butene}) = 9.37 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (Atkinson and Arey, 2003).

Preferred Values

$$k = 1.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

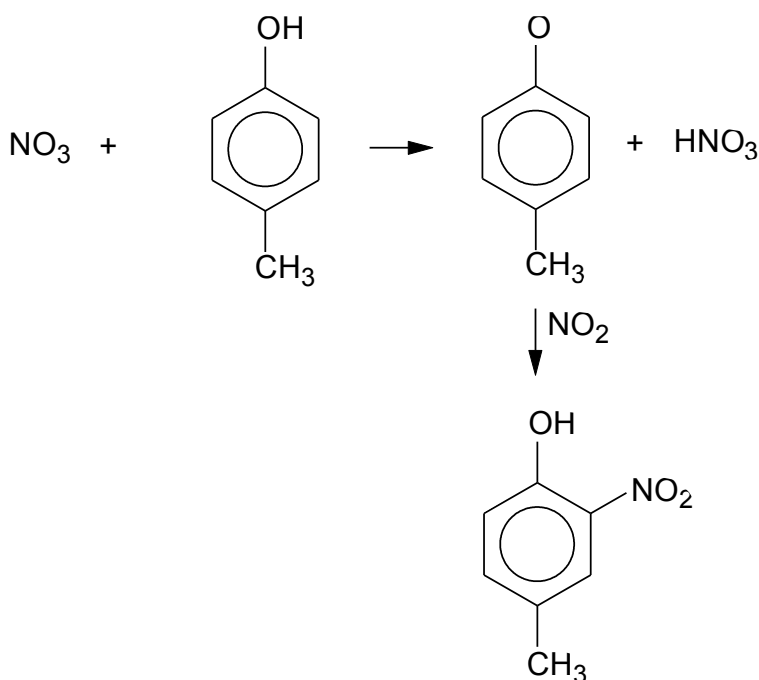
Reliability

$$\Delta \log k = \pm 0.15 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The reported rate coefficients are all from relative rate studies conducted at room temperature, and are in reasonable agreement. The rate coefficient of Carter et al. (1981) is subject to some uncertainties because of the concurrent reaction of O_3 with 2-methyl-2-butene. The preferred value is based on the study of Atkinson et al. (1992) in which the rate coefficient was measured relative to that for $NO_3 + 2\text{-methyl-2-butene}$ (a fairly reliably known rate coefficient) and used the thermal decomposition of N_2O_5 to generate NO_3 radicals.

Atkinson et al. (1992) observed the formation of 4-methyl-2-nitrophenol in $74 \pm 16\%$ yield. 4-Methyl-2-nitrophenol formation is believed to arise from methylphenoxy + NO_2 , and the measured 4-methyl-2-nitrophenol yield of Atkinson et al. (1992) therefore suggests that channel (1) accounts for at least $76 \pm 16\%$ of the overall reaction.



References

- Atkinson, R. and Arey, J.: *Chem. Rev.*, 103, 4605, 2003.
Atkinson, R., Aschmann, S. M., Arey, J.: *Environ. Sci. Technol.*, 26, 1397, 1992.
Atkinson, R., Carter, W. P. L., Plum, C. N., Winer, A. M. and Pitts Jr., J. N.: *Int. J. Chem. Kinet.*, 16, 887, 1984.
Carter, W. P. L., Winer, A. M. and Pitts Jr., J. N.: *Environ. Sci. Technol.*, 15, 829, 1981.
IUPAC: <http://iupac.pole-ether.fr> (2013).