IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_AROM2

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O_3 + $C_6H_5CH_3$ (toluene) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Relative Rate Coefficients			
$(1.2 \pm 0.6) \times 10^{-20}$	298 ± 2	Stedman and Niki, 1973	S-CL (a)
$(1.5 \pm 0.8) \times 10^{-22}$	297 ± 2	Pate et al., 1976	S-CL (a)
2.34×10^{-12} exp[-(6694 ± 403)/T]	298-398	Toby et al., 1985	S-UVA (b)
4.1 x 10^{-22}	298		

Comments

(a) Static system with chemiluminescence detection of O_3.
(b) Static system, with UV absorption detection of O_3 at 253.7 nm.

Preferred Values

$k < 1 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Comments on Preferred Values

The rate coefficient reported by Stedman and Niki (1973) is a factor of ~100 higher than the room temperature rate coefficients of Pate et al. (1976) and Toby et al. (1985). Moreover, Stedman and Niki (1973) observed no reaction of a mixture of xylene isomers with O_3, with $k < 5 \times 10^{-21}$ cm^3 molecule^{-1} s^{-1} at 298 ± 2 K; hence their rate coefficient for toluene appears to be erroneously high and is not used in the evaluation. The reaction of O_3 with toluene is slow and kinetic studies are subject to the influence of secondary reactions. Therefore, an upper limit to the rate constant is recommended which is consistent with the measured values of Pate et al. (1976) and Toby et al. (1985).

References

Pate, C. T., Atkinson, R. and Pitts Jr., J. N.: J. Environ. Sci. Health, A11, 1, 1976.
Stedman, D. H. and Niki, H.: Environ. Lett., 4, 303, 1973.
Toby, S., Van de Burgt, L. J. and Toby, F. S.: J. Phys. Chem., 89, 1982, 1985.