

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_AROM5

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This data sheet last evaluated September 2008; last change in preferred values September 2008.

O₃ + *p*-CH₃C₆H₄OH (*p*-cresol) → products

Rate coefficient data

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
~6 × 10 ⁻¹⁹	300 ± 1	Atkinson et al., 1978	S-GC (a)
(4.71 ± 0.66) × 10 ⁻¹⁹	296 ± 2	Atkinson et al., 1982	S-CL (b)

Comments

- (a) *p*-Cresol disappearance monitored by GC in the presence of excess O₃. Experiments were carried out in a ~5500 L Teflon chamber at atmospheric pressure of air. The cited rate was stated to be uncertain by a factor of ~2 and may be an upper limit due to the possibility of secondary reactions removing *p*-cresol.
- (b) O₃ decays were monitored by chemiluminescence in the presence of excess *p*-cresol in a ~175 L Teflon chamber at atmospheric pressure of air.

Preferred Values

$$k = 4.7 \times 10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

Reliability

$$\Delta \log k = \pm 0.3 \text{ at } 298 \text{ K.}$$

Comments on Preferred Values

The preferred value is based on the study of Atkinson et al. (1982) in which O₃ decays were monitored in the presence of excess *p*-cresol. The approximate rate coefficient of Atkinson et al. (1978), which may be an upper limit due to secondary reactions removing *p*-cresol, is reasonably consistent with that of Atkinson et al. (1982).

References

- Atkinson, R., Aschmann, S. M., Fitz, D. R., Winer, A. M. and Pitts Jr., J. N.: *Int. J. Chem. Kinet.*, 14, 13, 1982.
- Atkinson, R., Darnall, K. R. and Pitts Jr., J. N.: *J. Phys. Chem.*, 82, 2759, 1978.