

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox_AROM1

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O₃ + C₆H₆ (benzene) → products

Rate coefficient data

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	Temp./K	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>			
$(7 \pm 4) \times 10^{-23}$	297 ± 2	Pate et al., 1976	S-CL (a)
$1.05 \times 10^{-11} \exp[-(7398 \pm 353)/T]$	298-423	Toby et al., 1985	S-UVA (b)
1.7×10^{-22}	298		

Comments

- (a) Static system with chemiluminescence detection of O₃.
- (b) Static system, with UV absorption detection of O₃ at 253.7 nm.

Preferred Values

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

Comments on Preferred Values

The reaction of O₃ with benzene 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.
Toby, S., Van de Burgt, L. J. and Toby, F. S.: J. Phys. Chem., 89, 1982, 1985.