

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oBrOx9

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Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(6.0 \pm 0.4) \times 10^{-14}$	303	Brown et al., 1989, 1990	DF-RF
$1.28 \times 10^{-12} \exp[-(995 \pm 38)/T]$	298-460	Orkin and Khamaganov, 1993	DF-EPR
$(4.50 \pm 0.40) \times 10^{-14}$	298		

Preferred Values

$k = 4.6 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k = 1.2 \times 10^{-12} \exp(-970/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 290-460 K.

Reliability

$\Delta \log k = \pm 0.20$ at 298 K.

$\Delta(E/R) = \pm 300$ K.

Comments on Preferred Values

The rate coefficient of Brown et al. (1989, 1990) at 303 K is ~25% higher than that calculated from the Arrhenius expression of Orkin and Khamaganov (1993). A least-squares analysis of the rate coefficients of Orkin and Khamaganov (1993) leads to the preferred Arrhenius expression.

References

Brown, A. C., Canosa-Mas, C. E., Parr, A. D., Pierce, J. M. T. and Wayne, R. P.: Nature, 341, 635, 1989.

Brown, A. C., Canosa-Mas, C. E., Parr, A. D. and Wayne, R. P.: Atmos. Environ., 24A, 2499, 1990.

Orkin, V. L. and Khamaganov, V. G.: J. Atmos. Chem., 16, 169, 1993.