

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oBrOx4

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 updated: 29th March 2005.

HO + CF₃Br (Halon 1301) → products

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/Comments
<i>Absolute Rate Coefficients</i>			
$<1.2 \times 10^{-16}$	298	Burkholder et al., 1991	DF-LMR/PLP-LIF
$<2.0 \times 10^{-17}$	298	Orkin and Khamaganov, 1993	DF-EPR
$<4.0 \times 10^{-16}$	460		

Preferred Values

$k < 6.0 \times 10^{-18} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k < 1.0 \times 10^{-12} \exp(-3600/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 250-460 K.

Comments on Preferred Values

Only upper limits to the rate coefficients were observed in the studies of Burkholder et al. (1991) and Orkin and Khamaganov (1993). The A-factor for the reaction was estimated to be $\sim 1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The lower limit for E/R was estimated to be $>3600 \text{ K}$ based on the upper limit value of the rate coefficient determined by Orkin and Khamaganov (1993) at 460 K. The upper limit for the rate coefficient at 298 K is obtained using these parameters.

References

- Burkholder, J. B., Wilson, R. R., Gierczak, T., Talukdar, R., McKeen, S. A., Orlando, J. J., Vaghjiani, G. L. and Ravishankara, A. R.: J. Geophys. Res. 96, 5025, 1991.
Orkin, V. L. and Khamaganov, V. G.: J. Atmos. Chem. 16, 169, 1993.