

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oBrOx3

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HO + CHF₂Br (Halon 1201) → H₂O + CF₂Br

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/Comments
<i>Absolute Rate Coefficients</i>			
$4.4 \times 10^{-13} \exp[-(1050 \pm 400)/T]$ $(1.3 \pm 0.3) \times 10^{-14}$	275-420 298	Brown et al., 1990	DF-RF
$7.4 \times 10^{-13} \exp[-(1300 \pm 100)/T]$ $(1.06 \pm 0.08) \times 10^{-14}$	233-432 298	Talukdar et al., 1991	PLP-LIF/DF-LMR
$9.3 \times 10^{-13} \exp[-(1326 \pm 33)/T]$ $(1.10 \pm 0.09) \times 10^{-14}$	298-460 298	Orkin and Khamaganov, 1993	DF-EPR
<i>Relative Rate Coefficients</i>			
$6.11 \times 10^{-21} T^{2.82} \exp[-(527 \pm 31)/T]$ 9.9×10^{-15}	283-368 298	Hsu and DeMore, 1995	RR (a)

Comments

- (a) HO radicals were generated by the UV photolysis of O₃ in the presence of water vapor in O₃-H₂O-CHF₂Br-CH₄-O₂-N₂ mixtures. The concentrations of CHF₂Br and CH₄ were measured by FTIR spectroscopy. The measured rate coefficient ratio of $k(\text{HO} + \text{CHF}_2\text{Br})/k(\text{HO} + \text{CH}_4) = (0.33 \pm 0.03) \exp[(460 \pm 31)/T]$ is placed on an absolute basis by using a rate coefficient of $k(\text{HO} + \text{CH}_4) = 1.85 \times 10^{-20} T^{2.82} \exp(-987/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (IUPAC, current recommendation).

Preferred Values

$k = 1.0 \times 10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K.

$k = 7.9 \times 10^{-13} \exp(-1300/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 230-360 K.

Reliability

$\Delta \log k = \pm 0.10$ at 298 K.

$\Delta(E/R) = \pm 150 \text{ K}$.

Comments on Preferred Values

The absolute coefficients of Talukdar et al. (1991) and Orkin and Khamaganov (1993), and the relative rate data of Hsu and DeMore (1995) are in excellent agreement at 298 K. The absolute rate coefficients of Brown et al. (1990) are significantly higher and are not used in the evaluation. Above room temperature, the absolute rate coefficients of Talukdar et al. (1991) are lower than those of Orkin and Khamaganov (1993): at 430 K the rate coefficient of Talukdar et al. (1991) is 20% lower than that of Orkin and Khamaganov (1993). The data of Hsu and DeMore (1995) display a slightly higher temperature dependence than those observed in the absolute rate studies at temperatures up to 370 K.

The preferred 298 K rate coefficient is the mean of the absolute rate coefficients of Talukdar et

al. (1991), Orkin and Khamaganov (1993) and the relative rate coefficient Hsu and DeMore (1995). The temperature dependence is that measured by Talukdar et al. (1991), with the pre-exponential factor adjusted to fit the 298 K preferred value.

References

Brown, A. C., Canosa-Mas, C. E., Parr, A. D., Rothwell, K. and Wayne, R. P.: *Nature* 347, 541, 1990.

Hsu, K.-J. and DeMore, W. B.: *J. Phys. Chem.* 99, 1235, 1995.

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

Talukdar, R., Mellouki, A., Gierczak, T., Burkholder, J. B., McKeen, S. A. and Ravishankara, A. R.: *Science* 252, 693, 1991.