IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox2

This data sheet updated: 2nd October 2001.

$O + O_3 \rightarrow 2O_2$

$\Delta H^\circ = -391.9$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.1 \times 10^{-11} \exp(-2155/T)$	269-409	McCrumb and Kaufman, 1972[1]	(a)
$2.0 \times 10^{-11} \exp(-2280/T)$	220-353	Davis, Wong and Lephardt, 1973[2]	PLP-RF
8.3×10^{-15}	298	West, Weston and Flynn, 1978[3]	PLP-RF
$2.12 \times 10^{-11} \exp(-2337/T)$	262-335	Arnold and Comes, 1979[4]	FP-RA
$5.6 \times 10^{-12} \exp(-1959/T)$	220-377	Wine *et al*., 1983[5]	PLP-RF
8.26×10^{-15}	297		

Comments

(a) Flow system used, with O(^{3}P) atoms being produced by the pyrolysis of O_3.

Preferred Values

$k = 8.0 \times 10^{-15}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 8.0 \times 10^{-12} \exp(-2060/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 200-400 K.

Reliability

$\Delta \log k = \pm 0.08$ at 298 K.
$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The study of Wine *et al*.[5] yields values of k in close agreement with those from other studies, over the whole temperature range covered. Our preferred values are based on the least-squares expression obtained by Wine *et al*.[5] from a fit of their data plus those of McCrumb and Kaufman,[1] Davis *et al*.,[2] West *et al*.[3] and Arnold and Comes.[4] Computed rate constants[6] using variational transition state theory are in satisfactory agreement with the experimental results.

References

[1] J. L. McCrumb and F. Kaufman, J. Chem. Phys. **57**, 1270 (1972).
[2] D. D. Davis, W. Wong, and J. Lephardt, Chem. Phys. Lett. **22**, 273 (1973).
[3] G. A. West, R. E. Weston, Jr., and G. W. Flynn, Chem. Phys. Lett. **56**, 429 (1979).
[4] I. Arnold and F. J. Comes, Chem. Phys. **42**, 231 (1979).
[5] P. H. Wine, J. M. Nicovich, R. J. Thompson, and A. R. Ravishankara, J. Phys. Chem. **87**, 3948 (1983).
[6] N. Balakinshnan and G. D. Billing, Chem. Phys. Lett. **242**, 68 (1995).