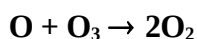


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox2

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: 2<sup>nd</sup> October 2001.



$$\Delta H^\circ = -391.9 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data

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

### Comments

- (a) Flow system used, with O(<sup>3</sup>P) atoms being produced by the pyrolysis of O<sub>3</sub>.

### Preferred Values

$k = 8.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

$k = 8.0 \times 10^{-12} \exp(-2060/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  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.*<sup>5</sup> 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.*<sup>5</sup> from a fit of their data plus those of McCrumb and Kaufman,<sup>1</sup> Davis *et al.*,<sup>2</sup> West *et al.*<sup>3</sup> and Arnold and Comes.<sup>4</sup> Computed rate constants<sup>6</sup> using variational transition state theory are in satisfactory agreement with the experimental results.

## References

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