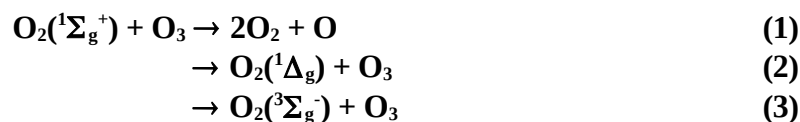


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet Ox10

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.



$$\Delta H^\circ(1) = -50.4 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(2) = -62.6 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(3) = -156.9 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data ( $k = k_1 + k_2 + k_3$ )

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.5 \pm 0.5) \times 10^{-11}$	295	Gilpin, Schiff and Welge, 1971 <sup>1</sup>	FP-CL (a)
$(2.3 \pm 0.5) \times 10^{-11}$	295	Snelling, 1974 <sup>2</sup>	FP (a)
$(2.2 \pm 0.2) \times 10^{-11}$	300	Slanger and Black, 1979 <sup>3</sup>	(a) (b)
$(1.8 \pm 0.2) \times 10^{-11}$	295	Amimoto and Wiesenfeld, 1980 <sup>4</sup>	FP-RA
$(2.2 \pm 0.3) \times 10^{-11}$	295-361	Choo and Leu, 1985 <sup>5</sup>	DF-CL (c)
$(1.96 \pm 0.09) \times 10^{-11}$	300	Shi and Barker, 1990 <sup>6</sup>	PLP-CL (d)
$(2.06 \pm 0.22) \times 10^{-11}$	300	Turnipseed <i>et al.</i> , 1991 <sup>7</sup>	PLP-RF (e)

### Comments

- $\text{O}_2(^1\Sigma_g^+)$  detected in emission.
- Flow system with  $\text{O}_2(^1\Sigma_g^+)$  being produced by the modulated photolysis of  $\text{O}_2$  at 147.0 nm to produce  $\text{O}(^1\text{D})$  atoms, followed by  $\text{O}(^1\text{D}) + \text{O}_2 \rightarrow \text{O}(^3\text{P}) + \text{O}_2(^1\Sigma_g^+)$ .
- Negligible temperature dependence was observed, with  $E/R < \pm 300$  K.
- $\text{O}_2(^1\Sigma_g^+)$  generated by the reaction  $\text{O}(^1\text{D}) + \text{O}_2 \rightarrow \text{O} + \text{O}_2(^1\Sigma_g^+)$ , with  $\text{O}(^1\text{D})$  atoms being produced from 308 nm pulsed laser photolysis of  $\text{O}_3$ .
- Rate coefficient for global reaction of  $\text{O}_2(^1\Sigma_g^+)$  with  $\text{O}_3$  was derived by modeling the temporal behavior of  $\text{O}(^3\text{P})$  and  $\text{O}(^1\text{D})$  atoms.

## Preferred Values

$k = 2.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ , independent of temperature over the range 295-360 K.  
 $k_1 = 1.5 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  at 298 K.

### Reliability

$\Delta \log k = \pm 0.06$  at 298 K.

$\Delta \log k_1 = \pm 0.10$  at 298 K.

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

### Comments on Preferred Values

The preferred value at 298 K is based on all of the studies cited in the table,<sup>1-7</sup> which show very good agreement at room temperature. The temperature independence reported in the study of Choo and Leu<sup>5</sup> is adopted in the evaluation. Channel (1) accounts for  $70 \pm 20\%$  of the total reaction.<sup>3,4</sup>

## References

- <sup>1</sup> R. Gilpin, H. I. Schiff, and K. H. Welge, *J. Chem. Phys.* **55**, 1087 (1971).
- <sup>2</sup> D. R. Snelling, *Can. J. Chem.* **52**, 257 (1974).
- <sup>3</sup> T. G. Slanger and G. Black, *J. Chem. Phys.* **70**, 3434 (1979).
- <sup>4</sup> S. T. Amimoto and J. R. Wiesenfeld, *J. Chem. Phys.* **72**, 3899 (1980).
- <sup>5</sup> K. Y. Choo and M.-T. Leu, *Int. J. Chem. Kinet.* **17**, 1155 (1985).
- <sup>6</sup> J. Shi and J. R. Barker, *Int. J. Chem. Kinet.* **22**, 1283 (1990).
- <sup>7</sup> A. A. Turnipseed, G. L. Vaghjiani, T. Gierczak, J. E. Thompson, and A. R. Ravishankara, *J. Chem. Phys.* **95**, 3244 (1991).