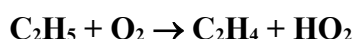


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet II.A4.88 R\_Oxygen3

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. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys. 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, (<http://iupac.pole-ether.fr>).

This data sheet last evaluated: June 2012; last change in preferred values: June 2012.



$$\Delta H^\circ = -54.1 \text{ kJ}\cdot\text{mol}^{-1}$$

### Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$<10^{-13}$	1000	Wagner et al., 1990	PLP-MS (a)
$1.61 \times 10^{-12}(T/298)^{-1.87}\exp(-707/T)$	296-700	DeSain et al., 2003	(b)
<i>Relative Rate Coefficients</i>			
$1.9 \times 10^{-14}$ (130 mbar, air)	298	Kaiser et al., 1990	(c)
$3.8 \times 10^{-15}$ (1 bar, air)	298		
$9.8 \times 10^{-16}$ (8 bar, air)	298		
$3.4 \times 10^{-13}\exp(-855/T)$	298-680	Kaiser, 2002	(d)

### Comments

- Experimental and theoretical study of the  $\text{C}_2\text{H}_5 + \text{O}_2$  reaction. Experiments were carried out in tubular flame reactor.  $\text{C}_2\text{H}_5$  radicals were formed by laser photolysis of  $\text{C}_2\text{H}_5\text{Br}$  or  $\text{CCl}_4\text{-C}_2\text{H}_6$  mixtures. Concentrations of  $\text{C}_2\text{H}_5$  and  $\text{C}_2\text{H}_4$  were monitored by photoionization MS.
- Pulsed photolytic Cl-initiated oxidation of ethane with time-resolved observation of OH by LIF. Detailed master equation modelling of the complex-forming bimolecular reaction. Partial suppression of the reaction with increasing pressure by collisional stabilization of  $\text{C}_2\text{H}_5\text{O}_2$ . The given rate coefficient corresponds to zero pressure.
- Study of the yields of  $\text{C}_2\text{H}_4$  produced relative to  $\text{C}_2\text{H}_6$  consumed (GC analysis) in a system in which  $\text{C}_2\text{H}_5$  radicals were generated by UV irradiation of  $\text{Cl}_2\text{-C}_2\text{H}_6\text{-O}_2\text{-N}_2$  (or air) mixtures. Up to 8 bar the percentage of  $\text{C}_2\text{H}_4$  produced, relative to the  $\text{C}_2\text{H}_6$  consumed, decreased from 12% to 0.02%, following a  $P^{(-0.8 \pm 0.1)}$  pressure dependence in air. The listed pressure-dependent  $k$  values are relative to values of  $k(\text{C}_2\text{H}_5 + \text{O}_2 + \text{M} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{M})$  calculated from Baldwin et al. (1980).
- Steady-state photolysis of  $\text{Cl}_2\text{-C}_2\text{H}_6\text{-O}_2$  mixtures at constant density of  $6.8 \times 10^{18} \text{ molecule cm}^{-3}$ . GC/MS analysis after irradiation.

## Preferred Values

$$k_0 = 1.5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K}$$

$$k_0 = 1.61 \times 10^{-12} (T/298)^{-1.87} \exp(-707/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the range } 298\text{-}700 \text{ K}$$

### Comments on Preferred Values

This is a chemical activation system for which HO<sub>2</sub> formation competes with collisional stabilization of C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> (see data sheet for C<sub>2</sub>H<sub>5</sub> + O<sub>2</sub> + M → C<sub>2</sub>H<sub>5</sub>O<sub>2</sub> + M). HO<sub>2</sub> yields decrease with increasing pressure and increase with increasing temperature. The preferred pressure-dependent values of *k* at 298 K are from the product study of Kaiser et al. (1990). The zero-pressure limiting rate coefficient is from DeSain et al. (2003). For a full discussion of the C<sub>2</sub>H<sub>5</sub> + O<sub>2</sub> reaction, see Wagner et al. (1990), DeSain et al. (2003), Carstensen et al. (2005), and Taatjes (2006). For atmospheric conditions the interaction of C<sub>2</sub>H<sub>5</sub> with O<sub>2</sub> predominantly leads to C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>.

## Preferred Values

Parameter	Value	T/K
$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.5 \times 10^{-13}$	298
$k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$1.6 \times 10^{-12} (T/300)^{-1.87} \exp(-707/T)$	298-700
$k(1 \text{ bar N}_2)/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$3.8 \times 10^{-15}$	298
<i>Reliability</i>		
$\Delta \log k_0$	± 0.5	298
$\Delta E_0/R$	± 300 K	298-700

## References

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