

# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet O<sub>x</sub>\_VOC4

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This data sheet last evaluated: 29<sup>th</sup> May 2008 (with no revision of the preferred values).

## O<sub>3</sub> + C<sub>2</sub>H<sub>2</sub> → products

### Rate coefficient data

<i>k</i> /cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
(7.8 ± 1.2) × 10 <sup>-21</sup>	294	Atkinson and Aschmann, 1984	S-CL (a)
4.13 × 10 <sup>-21</sup>	288	Du et al., 2006	S-UV (b)

### Comments

- (a) Static system, with [O<sub>3</sub>] being monitored by chemiluminescence in large excess of C<sub>2</sub>H<sub>2</sub> at a total pressure of 980 mbar.
- (b) C<sub>2</sub>H<sub>2</sub> measured by GC; no other details available.

### Preferred Values

$$k = 1 \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 298 \text{ K.}$$

#### Reliability

$$\Delta \log k = \pm 0.5 \text{ at } 298 \text{ K.}$$

#### Comments on Preferred Values

The literature data at room temperature (Cadle and Schadt, 1953; DeMore, 1969, 1971; Stedman and Niki, 1971; Pate et al., 1976; Atkinson and Aschmann, 1984, Du et al., 2006) exhibit a large degree of scatter, covering the range  $k = (0.41\text{-}7.8) \times 10^{-20} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ . The most recent studies of Atkinson and Aschmann (1984) and Du et al. (2006) give the lowest room temperature rate coefficients obtained to date, and are likely to be the most accurate since the presence of any impurities would have been likely to lead to higher values. Furthermore, the rate coefficients of Atkinson and Aschmann (1984) and Du et al. (2006) are in good agreement when allowance is made for the 6 K temperature difference in the two studies. The preferred value at 298 K is based upon the rate coefficients reported by Atkinson and Aschmann (1984) and Du et al. (2006) combined with an  $E/R$  of 5400-6000 K (DeMore, 1969; Chan et al., 2007). Because of the low magnitude of the rate coefficient, a large uncertainty is assigned to the preferred value.

There has been one study of the temperature dependence of the rate coefficient (DeMore, 1969) giving a value of  $E/R = 5435 \text{ K}$  over the temperature range 243-283 K. However, in view of the difficulties in studying this reaction and the small temperature range covered, no recommendation is made concerning the temperature dependence of this rate coefficient.

### References

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