IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet R_Oxygen_11

 This data sheet updated: 16th November 2006.

$CH_3CO + O_2 + M \rightarrow CH_3C(O)O_2 + M$

$\Delta H° = -162$ kJ·mol^{-1}

High-pressure rate coefficients
Rate coefficient data

k_∞/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.0 \pm 0.4) \times 10^{-12}$	298	McDade et al., 1982	(a)
$(5.4 \pm 1.9) \times 10^{-12}$	296	Kaiser and Wallington, 1995	RR (b)
$(5.7 \pm 1.9) \times 10^{-12}$	295 ± 2	Tyndall et al., 1997	RR (c)
$(5.9 \pm 1.9) \times 10^{-12}$	228		
$(4.4 \pm 0.7) \times 10^{-12}$	295	Sehested et al., 1998	PR-AS (d)
$(3.9 \pm 0.2) \times 10^{-12}$	295	Blitz et al., 2002	PLP-LIF (e)
$(5.7 \pm 0.1) \times 10^{-12}$	213		

Comments

(a) Flow system with CH_3CO generated from pulsed photolysis of CH_3COCH_3 or $CH_3COCH_2COCH_3$. [CH_3CO] was monitored by photoionization mass spectrometry and kinetics evaluated from pseudo-first-order decays of CH_3CO. The pressure range was 1.3 mbar to 5 mbar.

(b) Measurement of the rate coefficient ratio for $k(CH_3CO + Cl_2)/k(CH_3CO + O_2) = 7.9 \pm 0.5$ at 930 mbar total pressure. This rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of $k(CH_3CO + Cl_2) = (4.3 \pm 1.5) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Tyndall et al., 1999).

(c) Measurement of the rate coefficient ratios $k(CH_3CO + Cl_2)/k(CH_3CO + O_2)$ at 228 K and 298 K over the pressure range 0.13 mbar to 1460 mbar. The rate constant k was observed to increase with increasing pressure, with the rate coefficient k approaching the high-pressure limit above ~400 mbar. The rate coefficient ratio is placed on an absolute basis by use of a rate coefficient of $k(CH_3CO + Cl_2) = (4.3 \pm 1.5) \times 10^{-11}$ cm^3 molecule^{-1} s^{-1} (Tyndall et al., 1999).

(d) Pulse radiolysis of a mixture of CH_3CHO and O_2 in 1 bar of SF_6 coupled with transient UV absorption spectroscopy of $CH_3C(O)O_2$ at 260 nm. Numerical modelling is used in support of the complex reaction mechanism.

(e) Photolysis of acetone at 248 nm coupled to LIF detection of HO in the pressure range 13 to 550 mbar at 295K and 9 to 400 mbar at 213K. From the pressure dependence of the bimolecular rate constant and the absolute yield of HO the chemical activation mechanism and the zero-pressure HO formation channel have been confirmed. The yield of HO is approximately 10% at 550 mbar in the range 213 to 295K. Modelling confirms that k is approaching the high pressure limit at 550 mbar.

Preferred Values

$k_\infty = 5.1 \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}, independent of temperature over the range 220 to 300 K.

Reliability

$\Delta \log k_\infty = \pm 0.2$ over the temperature range 220 K to 300 K.

Comments on Preferred Values

The preferred values are based on the data of Sehested et al. (1998) and Tyndall et al. (1997) using the temperature independent reference rate constant for $CH_3CO + Cl_2$ of Tyndall et al. (1999). The work of Blitz et al. (2002) confirms the chemical activation mechanism and the zero-pressure HO forming reaction channel suggested by Tyndall et al. (1997).

References

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