IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx27

This data sheet last evaluated: June 2015; last change in preferred values: December 2007.

$Cl + CH_3CF_3$ (HFC-143a) $\rightarrow HCl + CH_2CF_3$

$\Delta H° = 18.0$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$< 1 \times 10^{-14}$	298	Hitsuda et al., 2001	PLP-LIF (a)
Relative Rate Coefficients			
$6.9 \times 10^{-12} \exp(-3720/T)$	281-368	Tschuikow-Roux et al., 1985	RR (b)
2.6×10^{-17}	298		
$(3.85 \pm 0.25) \times 10^{-17}$	296	Nielsen et al. (1994)	RR (c)

Comments

(a) Laser photolysis of HCl at 193 nm as Cl atom source. Both Cl($^2P_{3/2}$) and Cl($^2P_{1/2}$) detected by VUV-LIF.

(b) Cl atoms were generated by the photolysis of Cl_2. Product yield ratios were determined by GC and the the measured rate coefficient $k(Cl+CH_3CF_3)/k(CH_4) = 1.05 \exp(-2479/T)$ is placed on an absolute basis using $k(Cl + CH_4) = 6.6 \times 10^{-12} \exp(-1240/T)$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

(c) Cl atoms were generated by the photolysis of Cl_2 in the UV irradiation of CH_3CF_3 – CH_3CF_2Cl – Cl_2 in 920 mbar of N_2, or air, diluent. The measured rate coefficient ratio of $k(Cl + CH_3CF_3)/k(Cl + CH_3CF_2Cl) = 0.094 \pm 0.006$ was placed on an absolute basis using $k(Cl + CH_3CF_2Cl) = 4.1 \times 10^{-16}$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	3.2×10^{-17}	298
k /cm^3 molecule^{-1} s^{-1}	$8.4 \times 10^{-12} \exp(-3720/T)$	280-370
Reliability		
$\Delta \log k$	± 0.3	298
$\Delta(E/R)$	± 500	

Comments on Preferred Values

The recommended rate coefficient at room temperature is an average of the results of the relative rate studies of Tschuikow-Roux et al. (1985) and Nielsen et al. (1994). The temperature dependence is based upon the work by Tschuikow-Roux et al. (1985). The room temperature upper limit to *k* of Hitsuda et al. (2001) is consistent with the recommendation.

References

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 Atmosoheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr

Hitsuda, K., Takahashi, K., Matsumi, Y. and Wallington, T. J.: J. Phys. Chem. A, 105, 5131, 2001.

Nielsen, O. J., Gamborg, E., Sehested, J., Wallington, T. J. and Hurley, M. D.: J. Phys. Chem., 98, 9518, 1994.

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