IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx30

This data sheet updated: 29th March 2005.

$HO + CF_3CHO \rightarrow H_2O + CF_3CO$

$\Delta H° = -107.2$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$(1.1 \pm 0.7) \times 10^{-12}$	299 ± 3	Dóbé et al., 1989	DF-RF
$(6.5 \pm 0.5) \times 10^{-13}$	298 ± 2	Scollard et al., 1993	PLP-RF
Relative Rate Coefficients			
$(4.4 \pm 1.0) \times 10^{-13}$	298 ± 2	Scollard et al., 1993	RR (a)
$(4.8 \pm 0.3) \times 10^{-13}$	298 ± 2	Sellevåg et al., 2004	RR (b)
$(6.15 \pm 0.80) \times 10^{-13}$	296 ± 2	Sulbaek Andersen et al., 2004	RR (c,d)
$(6.93 \pm 0.81) \times 10^{-13}$	296 ± 2	Sulbaek Andersen et al., 2004	RR (c,e)

Comments

(a) HO radicals were generated by the photolysis of CH_3ONO (or C_2H_5ONO)-NO-CF_3CHO-CH_3COCH_3-air mixtures at 1 bar pressure. The concentrations of CF3CHO and CH_3COCH_3 were measured by GC and FTIR spectroscopy. The measured rate coefficient ratio of k(HO + CF_3CHO)/k(HO + CH_3COCH_3) = (2.43 ± 0.53) is placed on an absolute basis by use of a rate coefficient of k(HO + CH_3COCH_3) = 1.80×10^{-13} cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

(b) HO radicals were generated by the photolysis of O_3 in the presence of H_2 at 1 bar pressure. FTIR was used to monitor the disappearance of reactant and reference compound. The measured rate coefficient ratio of k(HO + CF_3CHO)/k(HO + C_2H_6) = (2.00 ± 0.13) is placed on an absolute basis by use of a rate coefficient of k(HO + C_2H_6) = 2.4×10^{-13} cm^3 molecule^{-1} s^{-1} (IUPAC, current recommendation).

(c) HO radicals were generated by the photolysis of CH_3ONO in the presence of NO in air at a pressure of 933 mbar. The concentrations of CF_3CHO, C_2H_2, C_2H_4 and reaction products were measured by FTIR spectroscopy. The measured rate coefficient ratios k(HO + CF_3CHO)/k(HO + C_2H_2) and k(HO + CF_3CHO)/k(HO + C_2H_4) were placed on an absolute basis by using k(HO + C_2H_2) = 8.45×10^{-13} cm^3 molecule^{-1} s^{-1} at 296 K (Sørensen et al. 2003), and k(HO + C_2H_4) = 8.52×10^{-12} cm^3 molecule^{-1} s^{-1} at 296 K (Calvert et al. 2000).

(d) Relative to C_2H_2.

(e) Relative to C_2H_4.

Preferred Values

$k = 5.7 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1} at 298 K.

Reliability

$\Delta \log k = \pm 0.2$ at 298 K.

Comments on Preferred Values

The preferred 298 K rate coefficient is the average of the absolute and relative rate coefficients of Sulbaek Andersen et al., 2004, Sellevåg et al. (2004) and Scollard et al. (1993). The rate coefficient data of Dóbé et al. (1989) was not used due to its large uncertainty.

References

Calvert, J. G., Atkinson, R., Kerr, J. A., Madronich, S., Moortgat, G. K., Wallington, T. J., and Yarwood, G.: The Mechanism of Atmospheric Oxidation of the Alkenes, Oxford University Press, New York, 2000.

Dóbé, S., Khachatryan, L. A. and Berces, T.: Ber. Bunsenges. Phys. Chem. 93, 847, 1989.

IUPAC: http://iupac.pole-ether.fr, 2013.

Scollard, D. J., Treacy, J. J., Sidebottom, H. W., Balestra-Garcia, C., Laverdet, G., Le Bras, G., Mac Leod, H. and Téton, S.: J. Phys. Chem. 97, 4683, 1993.

Sellevåg, S. R., Kelly, T., Sidebottom, H. and Nielsen, C. J.: Phys. Chem. Chem. Phys. 6, 1243, 2004.

Sørensen, M., Kaiser, E. W., Hurley, M. D., Wallington, T. J. and Nielsen, O. J.: Int. J. Chem. Kinet. 35, 191, 2003.

Sulbaek Andersen, M. P., Nielsen, O. J., Hurley, M. D., Ball, J. C., Wallington, T. J., Stevens, J. E., Martin, J. W., Ellis, D. A. and Mabury, S. A.: J. Phys. Chem. A., 108, 5189, 2004.