IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx115

This data sheet last evaluated: June 2017; last change in preferred values: June 2017.

HO + E-$CF_3CH=CHF$ (HFO-1234ze(E)) → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
See comment (a)	220-370	Orkin et al., 2010	FP-RF (a)
$(7.11\pm 0.05) \times 10^{-13}$	298		
Relative Rate Coefficients			
$(8.00\pm0.82) \times 10^{-13}$	296	Søndergaard et al. 2007	RR (b)
$(8.72\pm0.47) \times 10^{-13}$	296		

Comments

(a) HO radicals were generated by the photolysis of H_2O by a xenon flash lamp in 30-200 Torr (40-267 mbar) of argon diluent. HO radicals were monitored using resonance fluorescence. There was no discernable (<5%) effect of total pressure over the range studied on the rate of reaction. A small but distinct curvature was evident in the Arrhenius plot and a modified Arrhenius expression, $k = 1.115 \times 10^{-13} (T/298)^{2.03} \exp(552/T)$ cm^3 molecule^{-1} s^{-1} was used to best represent the data.

(b) Photolysis of CH_3ONO in 700 Torr (933 mbar) of air diluent was used to generate HO radicals. The loss of $CF_3CH=CHF$ was measured relative to those of C_2H_2 and C_2H_4 and used to measure the rate coefficient ratios $k(CF_3CH=CHF)/k(C_2H_2) = 1.07\pm0.11$ and $k(CF_3CH=CHF)/k(C_2H_2) = 0.111\pm0.006$. Using $k(HO + C_2H_2) = 7.47 \times 10^{-13}$ and $k(HO + C_2H_4) = 7.85 \times 10^{-12}$ (Atkinson et al., 2006) gives $k(HO + CF_3CH=CHF) = (8.00\pm0.82) \times 10^{-13}$ and $(8.72\pm0.47) \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	7.11×10^{-13}	298
k /cm^3 molecule^{-1} s^{-1}	$6.21 \times 10^{-12} \exp(36/T)$	220-300
Reliability		
$\Delta \log k$	± 0.10	298
Δ E/R	± 100	220-300

Comments on Preferred Values

There is an approximately 15-20% difference between the room temperature rate coefficients measured in the relative rate study by Søndergaard et al. (2007) and the absolute rate study by Orkin et al. (2010). The difference in results is at the limit of the likely combined experimental uncertainties in the two studies. The k(298K) recommendation is based on the absolute rate study by Orkin et al. (2010). There was no discernible effect of total pressure over the range 30-200 Torr indicating that the reaction is at, or near, the high pressure limit for pressures above 30 Torr. The precision of the absolute rate measurements reveal a small curvature in the Arrhenius plot. A fit of a modified Arrhenius expression to the data set from Orkin et al. (2010) gives $k = 1.12 \times (T/298)^{2.03} \exp(551/T)$ cm^3 molecule^{-1} s^{-1}. A fit of the Arrhenius expression to the data below 300 K gives $k = 6.21 \times 10^{-12} \exp(36/T)$ cm^3 molecule^{-1} s^{-1}. While the modified Arrhenius expression provides a better representation of the measured data, for simplicity and consistency within the IUPAC recommended database we recommend the simple Arrhenius expression. The HO radical initiated oxidation of $CF_3CH=CHF$ gives $CF_3C(O)H$ and HC(O)F as products (Javadi et al., 2008).

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

Orkin, V. L.; Martynova, L. E.; and Ilichev, A. N. : J. Phys. Chem. A, 114, 5967, 2010.

Søndergaard, R.; Nielsen, O. J.; Hurley, M. D.; Wallington, T. J.; and Singh, R. : Chem. Phys. Lett., 443, 199, 2007.

Javadi, M. S. ; Søndergaard, R. ; Nielsen, O. J. ; Hurley, M. D. ; and Wallington, T. J. : Atmospheric Chemistry and Physics, 8, 3141, 2008.