IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx97; VII.A5.16

$$HO + CHF_2CHO \quad \rightarrow CHF_2CO + H_2O \qquad (1)$$
$$\rightarrow CF_2CHO + H_2O \qquad (2)$$

Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(1.7 \pm 0.2) \times 10^{-12}$	298	Scollard et al. (1993)	PLP-RF (a)
Relative Rate Coefficients			
$(1.32 \pm 0.28) \times 10^{-12}$	298	Scollard et al. (1993)	RR (b)
$(1.79 \pm 0.05) \times 10^{-12}$	298	Sellevåg et al. (2005)	RR (c)

Comments

(a) HO radicals were generated by the photolysis of nitric acid in argon at 15-100 Torr (20 - 133 mbar) pressure.

(b) HO radicals were generated by the photolysis of CH_3ONO (or C_2H_5ONO) in CH_3ONO (or C_2H_5ONO)-NO-CHF_2CHO-toluene-air mixtures at 730-750 Torr (973 - 1000 mbar) pressure. The concentrations of CHF_2CHO and toluene were measured by GC and/or FTIR spectroscopy. Scollard et al. (1993) did not report a value for the rate coefficient ratio k(HO + CHF_2CHO)/k(HO + toluene). Dividing the reported value of k(HO + CHF_2CHO) by the value of k(HO + toluene) used by Scollard et al. (1993) gives k(HO + CHF_2CHO)/k(HO + toluene) = 0.235 ± 0.005 which is placed on an absolute basis in the table above using k(HO + toluene) = 5.6×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (IUPAC, 2010).

(c) HO radicals were generated by the photolysis of O_3 in the presence of H_2 in 1013 mbar of air diluent. Propane was used as the reference compound. The concentrations of CHF_2CHO and propane were measured by FTIR spectroscopy and a rate coefficient ratio of k(HO + CHF_2CHO)/k(HO + propane) = 1.626 ± 0.042 was reported. Placing this result on an absolute basis using k(HO + propane) = 1.1×10^{-12} cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006) gives k(HO + CHF_2CHO) = $(1.79 \pm 0.05) \times 10^{-12}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.6×10^{-12}	298
Reliability		
$\Delta \log k$	0.15	298

Comments on Preferred Values

The results from the relative and absolute rate studies by Scollard et al. (1993) and Sellevåg et al. (2005) are in agreement within the likely combined experimental uncertainties. An average

of the results from Scollard et al. (1993) and Sellevåg et al. (2005) gives the recommended value of k(OH+CHF$_2$CHO) = 1.6×10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K. The reaction probably proceeds predominately via abstraction of the aldehydic hydrogen (channel 1) to give CHF$_2$C(O) radicals.

References

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