IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx83; VII.A1.12

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HO + $CHF_2(CF_2)_4CF_3$ (HFC-52-13p) → $CF_2(CF_2)_4CF_3$ + H_2O

Rate coefficient data (k)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
7.36×10^{-12} exp[-(1820 ± 60)/T]	250-430	Chen et al. (2004)	FP-LIF/ PLP-LIF (a)
$(1.69 \pm 0.07) \times 10^{-15}$	298		FP-LIF (b)
$(1.72 \pm 0.07) \times 10^{-15}$	298		PLP-LIF (c)
Relative Rate Coefficients			
4.87×10^{-13} exp[-1661/T]	253-328	Chen et al. (2004)	RR (d)
1.87×10^{-15}	298		
2.61×10^{-13} exp[-1422/T]	253-328	Chen et al. (2004)	RR (e)
2.28×10^{-15}	298		

Comments

(a) Experiments were conducted using two different absolute rate methods. Substantial care was taken to assure the purity of the sample. The sample of $CHF_2(CF_2)_4CF_3$ was purified using a GC with the middle fraction retained for experiments and was determined to be 99.998% pure. In the FP-LIF experiments the HO radicals were produced by the photolysis of H_2O using a Xe flash lamp and experiments were performed in 20-100 Torr (27-133 mbar) of argon bath gas. In the PLP-LIF experiments the HO radicals were produced by the photolysis of N_2O using a ArF excimer giving $O(^1D)$ atoms which react with H_2O laser flash lamp and experiments were performed in 20-100 Torr (27-133 mbar) of either argon or helium bath gas. The Arrhenius expression is that given by Chen et al. (2004) from a fit to the absolute rate data.

(b) Result obtained using FP-LIF technique at 298 K in 40-100 Torr (53-133 mbar) total pressure of argon bath gas.

(c) Result obtained using PLP-LIF technique at 298 K in 40-100 Torr (53-133 mbar) total pressure of argon or helium bath gas.

(d) Relative rate method with HO radicals produced by the 254 nm photolysis of O_3 in the presence of H_2O vapor in 200-500 Torr (267-665 mbar) of helium diluent. CHF_2Cl was used as a reference compound. The rate coefficient ratios $k(HO+CHF_2(CF_2)_4CF_3)/k(HO+CHF_2Cl)$ were placed on an absolute basis using $k(HO+CHF_2Cl) = 7.9 \times 10^{-13}$ exp(-1530/T) cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008).

(e) Relative rate method with HO radicals produced by the 254 nm photolysis of O_3 in the presence of H_2O vapor in 200-500 Torr (267-665 mbar) of helium diluent. CH_2FCF_3 was used as a reference compound. The rate coefficient ratios $k(HO+CHF_2(CF_2)_4CF_3)/k(HO+CH_2FCF_3)$ were placed on an absolute basis using $k(HO+CH_2FCF_3) = 4.9 \times 10^{-13}$ exp(-1395/T) cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2008).

Preferred Values

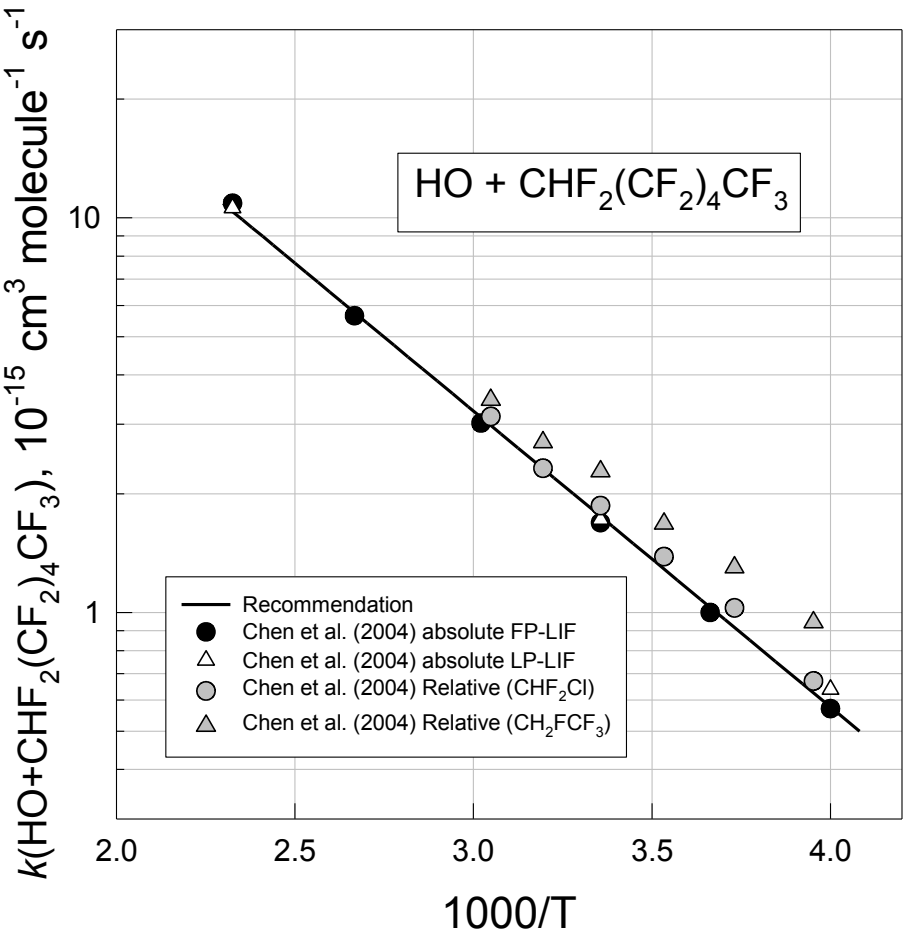
Parameter	Value	*T*/K
k /cm^3 molecule^{-1} s^{-1}	1.8×10^{-15}	298
k /cm^3 molecule^{-1} s^{-1}	5.76×10^{-13} exp (-1726/T)	250-430
Reliability		
$\Delta \log k$	0.10	298
Δ E/R	± 300	250-430

Comments on Preferred Values

The results obtained using two absolute rate methods by Chen et al. (2004) are in good agreement. An Arrhenius fit to the absolute rate data reported by Chen et al. (2004) with $1/k^2$ weighting of the data points gives $k(HO+CHF_2(CF_2)_4CF_3) = 5.76 \times 10^{-13}$ exp (-1726/T) cm^3 molecule^{-1} s^{-1} which is recommended. The relative rate experiments using CHF_2Cl reference are in excellent agreement with the results from the absolute rate study. The relative rate experiments using CH_2FCF_3 reference lie somewhat above, but are consistent within the experimental uncertainties with the recommended values.

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 8, 4141, 2008; IUPAC Subcommittee for Gas Kinetic Data Evaluation, http://www.iupac-kinetic.ch.cam.ac.uk. Chen, L., Tokuhashi, K., Kutsuna, S., and Sekiya, A.: Int. J. Chem. Kinet., 36, 26, 2004.


HO + CHF2(CF2)4CF3
Recommendation
Chen et al. (2004) absolute FP-LIF
Chen et al. (2004) absolute LP-LIF
Chen et al. (2004) Relative (CHF2Cl)
Chen et al. (2004) Relative (CH2FCF3)
k(HO+CHF2(CF2)4CF3), 10-15 cm3 molecule-1 s-1
10
1
2.0
2.5
3.0
3.5
4.0
1000/T