IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oFOx17

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HO + CH_2FCH_2F (HFC-152) → H_2O + CH_2FCHF

$\Delta H°$ = -69.5 kJ mol^{-1}

Rate coefficient data

k/cm^3 $molecule^{-1}$ s^{-1}	Temp./K	Reference	Technique/Comments
(1.12 ± 0.12) x 10^{-13}	298	Martin and Paraskevopoulos, 1983	FP-RA
5.11 x 10^{-12} exp [-(1190 ± 106)/T]	298-480	Kozlov et al., 2003	FP-RF
1.02 x 10^{-12} exp [-(706 ± 70)/T]	210-298		
(9.92 ± 0.18) x 10^{-14}	298		
Relative Rate Coefficients-			
4.77 x 10^{-18} T^2 exp [-(454 ± 23)/T]	293-397	Wilson et al., 2003	RR (a,b)
9.23 x 10^{-14}	298		
2.15 x 10^{-18} T^2 exp [-(188 ± 29)/T]	287-409	Wilson et al., 2003	RR (a,c)
1.02 x 10^{-13}	298		
4.68 x 10^{-18} T^2 exp [-(441 ± 16)/T]	292-393	Wilson et al., 2003	RR (a,d)
9.46 x 10^{-14}	298		

Comments

(a) Relative rate method. HO radicals were generated by photolyzing H_2O vapour at 185 nm. Reactant and reference compound concentrations were monitored by GC/MS.

(b) Relative to C_2H_6. An Arrhenius plot of the data gives the temperature dependence of the measured ratios as (0.32 ± 0.02) exp[(45 ± 23)/T], which is placed on an absolute basis using a rate coefficient of k(HO + C_2H_6) = 1.49 x 10^{-17} T^2 exp(-499/T) cm^3 $molecule^{-1}$ s^{-1} (IUPAC, current recommendation).

(c) Relative to cyclopropane. An Arrhenius plot of the data gives the temperature dependence of the measured ratios as (0.51 ± 0.04) exp[(266 ± 29)/T]], which is placed on an absolute basis using a rate coefficient of k(HO + cyclopropane) = 4.21 x 10^{-18} T^2 exp(-454/T) cm^3 $molecule^{-1}$ s^{-1} (Atkinson, 2003).

(d) Relative to CH_3CHF_2. An Arrhenius plot of the data gives the temperature dependence of the measured ratios as (1.67 ± 0.08) exp[(139 ± 16)/T], which is placed on an absolute basis using a rate coefficient of k(HO + CH_3CHF_2) = 2.80 x 10^{-18} T^2 exp(-580/T) cm^3 $molecule^{-1}$ s^{-1} (IUPAC, current recommendation).

Preferred Values

k = 1.0 x 10^{-13} cm^3 $molecule^{-1}$ s^{-1} at 298 K.

k = 1.5 x 10^{-12} exp(-800/T) cm^3 $molecule^{-1}$ s^{-1} over the temperature range 210-300 K.

Reliability

$\Delta \log k$ = ± 0.3 at 298 K.

$\Delta(E/R) = \pm 200$ K.

Comments on Preferred Values

The absolute rate coefficients of Kozlov et al. (2003) and the relative rate coefficients of Wilson et al. (2003) (relative to C_2H_6 and CH_2FCH_2F) are in good agreement over the temperature range (298–380 K). The absolute rate coefficient of Martin and Paraskevopoulos (1983) at 298 K agrees to within 20% or better to the data of Kozlov et al. (2003) and Wilson et al. (2003) (relative to C_2H_6 and CH_3CHF_2). The rate coefficients of Wilson et al. (2003) relative to cyclopropane exhibit a lower temperature dependence compared with the data of Kozlov et al. (2003) and the two other relative rate studies performed by Wilson et al. (2003). This may be due to the literature rate coefficient for HO + cyclopropane being not well established because of substantial scatter in the literature data. Therefore, the rate coefficients of Wilson et al. (2003) relative to cyclopropane were not used in the evaluation.

The absolute rate coefficients of Kozlov et al. (2003) and Martin and Paraskevopoulos (1983), and the relative rate coefficients of Wilson et al. (2003) relative to C_2H_6 and CH_3CHF_2 have been fitted to the three parameter equation $k = CT^2 \exp(-D/T)$ resulting in $k = 3.39 \times 10^{-18} T^2 \exp(-312/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 210-480 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 245 K and is derived from the three-parameter equation with $A = C e^2 T^2$ and $B = D + 2T$.

References

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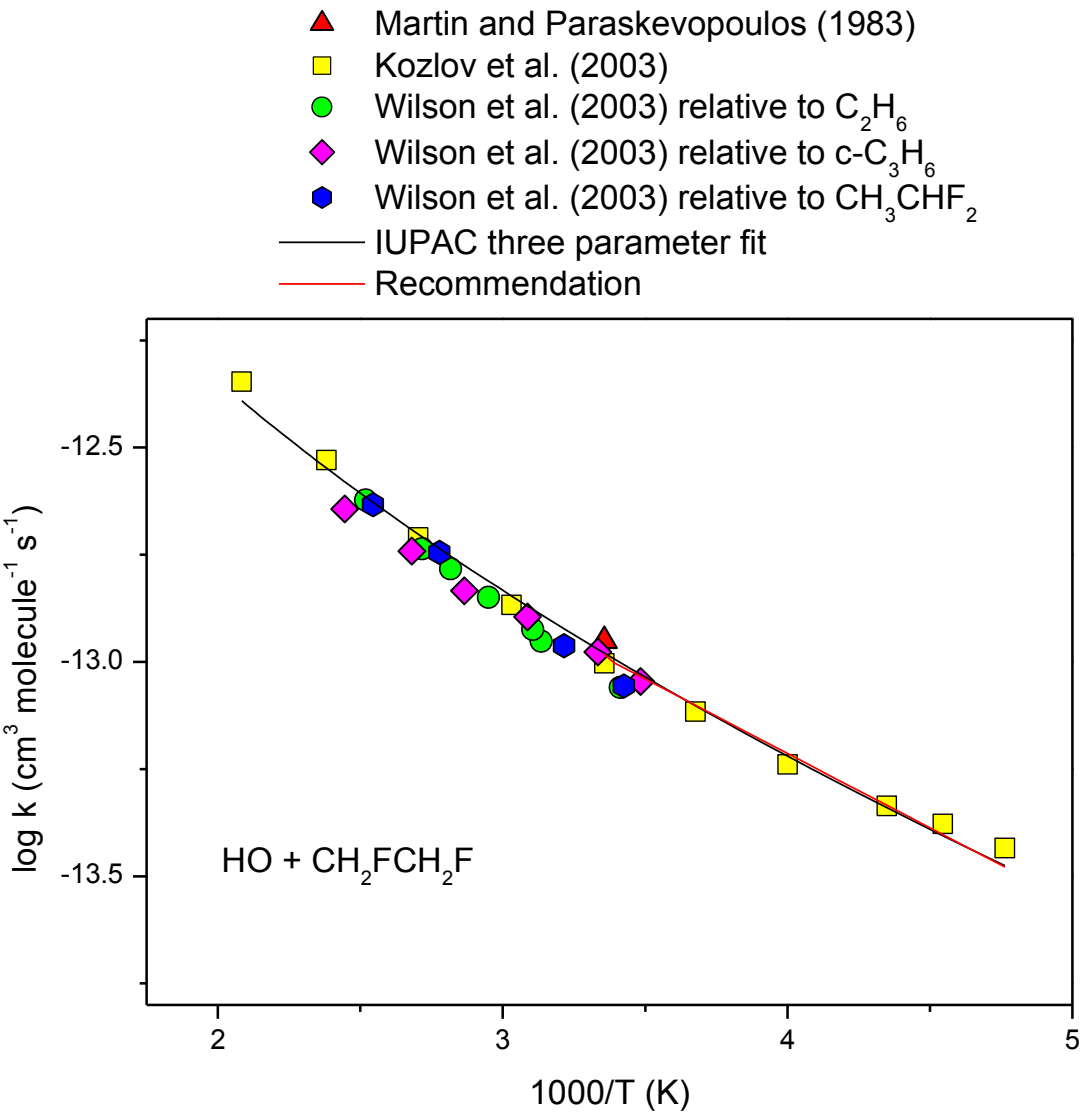
Kozlov, S. N., Orkin, V. L. and Kurylo, M. J.: J. Phys. Chem. A. 107, 2239, 2003.

Martin, J.-P. and Paraskevopoulos, G.: Can. J. Chem. 61, 861, 1983.

Wilson, E. W., Jr., Jacoby, A. M., Kukta, S. J., Gilbert, L. E. and DeMore, W. B.: J. Phys. Chem. A. 107, 9357, 2003.

Wilson, E. W., Jr., Sawyer, A. A. and Sawyer, H. A.: J. Phys. Chem. A. 105, 1445, 2001.


Martin and Paraskevopoulos (1983)
Kozlov et al. (2003)
Wilson et al. (2003) relative to C2H6
Wilson et al. (2003) relative to c-C3H6
Wilson et al. (2003) relative to CH3CHF2
IUPAC three parameter fit
Recommendation
HO + CH2FCH2F
log k (cm3 molecule-1 s-1)
1000/T (K)
-12.5
-13.0
-13.5
2
3
4
5