IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet SOx79

This data sheet last evaluated: June 2011; last change in preferred values: June 2011.

$HO + SO_2F_2 \rightarrow$ products (1)

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients, k			
$< 1 \times 10^{-15}$	294	Dillon et al., 2008	LP-LIF (a)
Relative Rate Coefficients			
$< 1 \times 10^{-16}$	296-333	Papadimitriou et al., 2008	(b)
$< 1.7 \times 10^{-14}$	298	Andersen et al., 2009	(c)

Comments

(a) 248 nm photolysis of H_2O_2 as HO source. Decay of HO attributed at least in part to reaction with impurities, hence the upper limit to k.

(b) 248 nm photolysis of O_3 / H_2O used as HO source. Depletion of SO_2F_2 and CHF_3 (reference reactant) was monitored by FTIR. Although some loss of SO_2F_2 was observed, the lack of a temperature dependence led the authors to suggest that this was due to reaction with $O(^1D)$. The upper limit to k was calculated using $k(HO + CHF_3) = 6.3 \times 10^{-13}\exp(2300/T)$ cm^3 molecule^{-1} s^{-1}.

(c) Photolysis of CH_3ONO in air as HO source. Depletion of SO_2F_2 and C_2H_2 (reference reactant) was monitored by FTIR to derive $k(HO + SO_2F_2) / k(HO + C_2H_2) < 0.02$. This was converted to an upper limit for k using $k(HO + C_2H_2) = 8.5 \times 10^{-13}$ cm^3 molecule^{-1} s^{-1}.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	$< 10^{-16}$	200-330 K

Comments on Preferred Values

All she studies of this reaction confirm that it is very slow. We adopt the experimental upper limit of Papadimitriou et al., 2008 for the preferred value. The thermochemical calculations of Papadimitriou et al., 2008 also suggest that the rate coefficient will however be considerably smaller at lower temperatures.

References

Dillon, T. J., Horowitz, A. and Crowley, J. N.: Atmos. Chem. Phys. 8, 1547-1557, 2008.

Papadimitriou, V. C., Portmann, R. W., Fahey, D. W., Muhle, J., Weiss, R. F. and Burkholder, J. B.: J. Phys. Chem. A 112, 12657-12666, 2008.
Andersen, M. P. S., Blake, D. R., Rowland, F. S., Hurley, M. D. and Wallington, T. J.: Env. Sci. Tech. 43, 1067-1070, 2009.