IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx55

 The citation for this data sheet is: 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., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.
This data sheet last evaluated: June 2015; last change in preferred values: November 2003.

HO + $CHFClCF_2Cl$ (HCFC-123a) → H_2O + $CFClCF_2Cl$

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$9.2 \times 10^{-13} \exp[-(1281 \pm 85)/T]$	298-460	Orkin and Khamaganov, 1993	DF-EPR
$(1.23 \pm 0.10) \times 10^{-14}$	298		

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.2×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	$8.4 \times 10^{-13} \exp(-1255/T)$	298-460
Reliability		
$\Delta \log k$	± 0.30	298
$\Delta(E/R)$	± 400	298-460

Preferred Values

$k = 1.2 \times 10^{-14}$ cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 8.4 \times 10^{-13} \exp(-1255/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 298-460 K.

Reliability

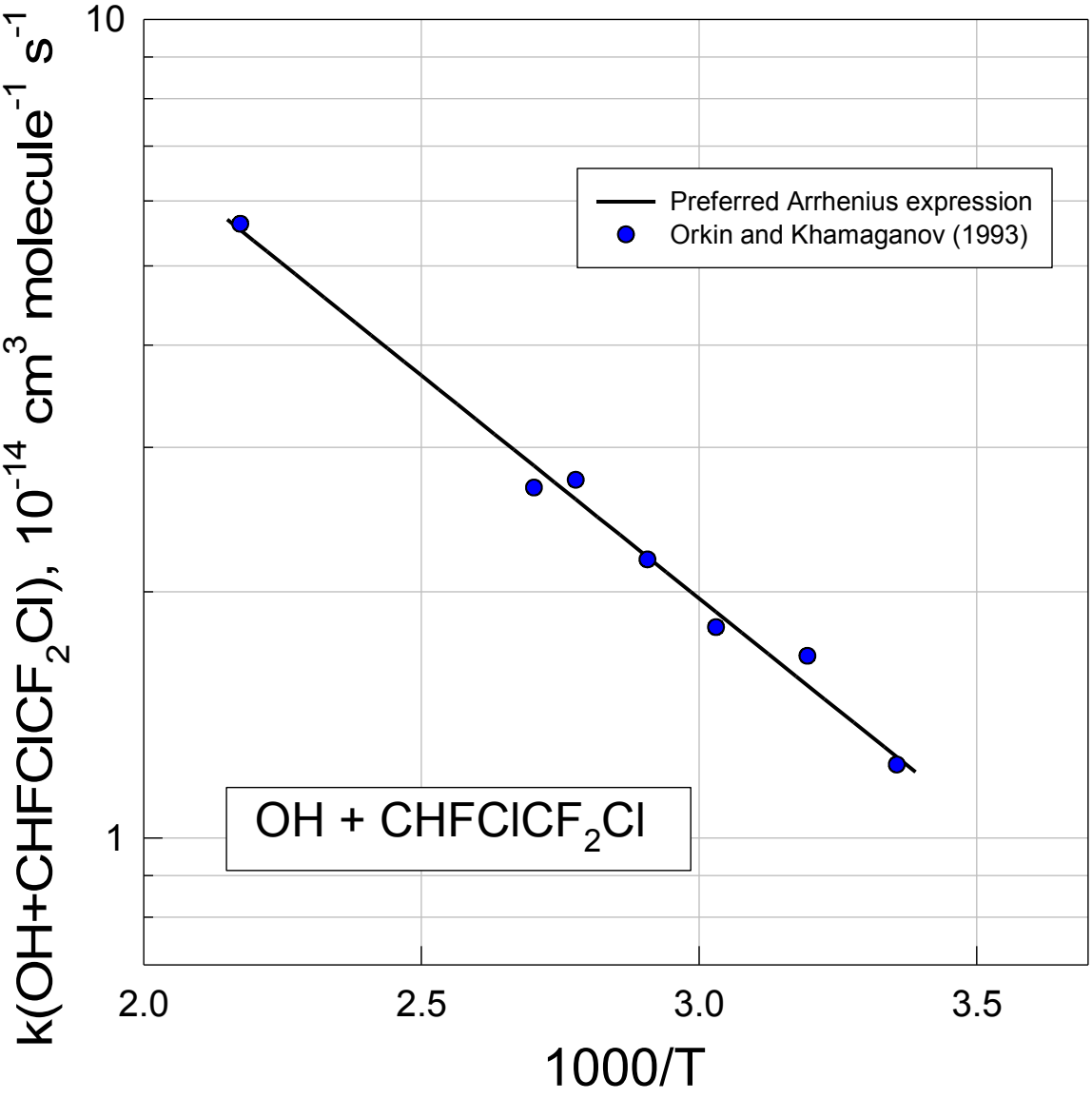
$\Delta \log k = \pm 0.3$ at 298 K.
$\Delta(E/R) = \pm 400$ K.

Comments on Preferred Values

The preferred Arrhenius expression is obtained from a unit-weighted least-squares analysis of the absolute rate coefficients of Orkin and Khamaganov (1993), the sole study conducted to date.

References

Orkin, V. L. and Khamaganov, V. G.: J. Atmos. Chem., 16, 157, 1993.


10
1
2.0
2.5
3.0
3.5
1000/T
k(OH+CHFClCF2Cl), 10-14 cm3 molecule-1 s-1
Preferred Arrhenius expression
Orkin and Khamaganov (1993)
OH + CHFClCF2Cl