IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet iFOx8

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., and Troe, J.: Atmos. Chem. Phys., 7, 891, 2007; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr.
This datasheet last evaluated: June 2014; last change in preferred values: September 2003.

$F + O_3 \rightarrow FO + O_2$

$\Delta H° = -113$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$2.8 \times 10^{-11} \exp[-(226 \pm 200)/T]$	253-365	Wagner, et al., 1972	DF-MS (a)
1.3×10^{-11}	298		
$(6.2 \pm 0.3) \times 10^{-12}$	298	Bedzhanyan, et al., 1993	DF-LMR (b)

Comments

(a) MS detection of O_3 decay in the presence of an excess of F atoms. The temporal profiles of F, FO, and O_3 were monitored by MS.
(b) Discharge flow system with excess of O_3 over F atoms. Rate of formation of FO radicals was monitored by LMR.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	1.0×10^{-11}	298
k /cm^3 molecule^{-1} s^{-1}	$2.2 \times 10^{-11} \exp(-230/T)$	250-370
Reliability		
$\Delta \log k$	± 0.25	298
Δ E/R	± 200	

Comments on Preferred Values

The preferred room temperature value is the average of the 298 K values from the two studies of Wagner et al. (1972) and Bedzhanyan et al. (1992). The temperature dependence is taken from Wagner et al. (1972) and the A-factor is fitted to the preferred 298 K value. The preferred value at room

temperature is supported by values of k derived indirectly in studies of the reactions of CF_3O and CF_3O_2 radicals with O_3 by Nielsen and Sehested (1993) and Maricq and Szente (1993).

References

Bedzhanyan, Yu. R., Markin, E. M. and Gershenzon, Yu. M.: Kinet. Catal. 33, 594, 1993; original pages 744-752, 1992.

Maricq, M. M. and Szente, J. J.: Chem. Phys. Lett. 213, 449, 1993.

Nielsen, O. J. and Sehested, J.: Chem. Phys. Lett. 213, 433, 1993.

Wagner, H. Gg., Zetzsch, C. and Warnatz, J: Ber. Bunsenges. Phys. Chem. 76, 526, 1972.